

CHEM 416: CHEMICAL REACTION ENGINEERING II

**INTRODUCTION TO REACTOR
DESIGN**





LEARNING OBJECTIVES

- At the end of this week's lecture, students should be able to:
 - Understand the essentials of reactor design.
 - Differentiate between a batch, steady-state flow and unsteady state flow reactors
 - Know the symbols and relationships between C_A and X_A



ESSENTIALS OF REACTOR DESIGN

- The focus of reactor design are
 - Knowing the size of the reactor, and
 - The type of reactor and
 - The best method of operation.
- Factors of importance in reactor design include:
 - The reacting conditions in the reactor
 - The time taken for the reaction to occur
 - The temperature,
 - The composition of the reacting fluid
 - The thermal character of the reaction, either endothermic or exothermic, the rate of heat addition or removal from the system, and
 - The flow pattern of fluid through the vessel.
- All these factors must be accounted for in predicting the performance of a reactor

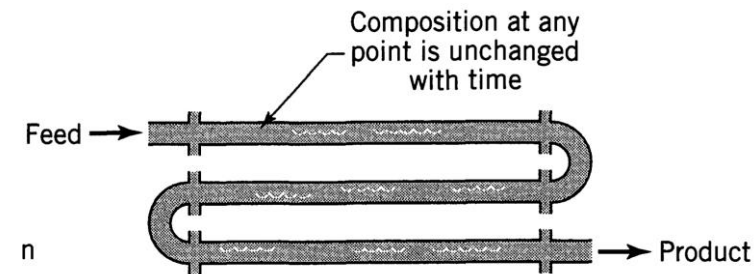
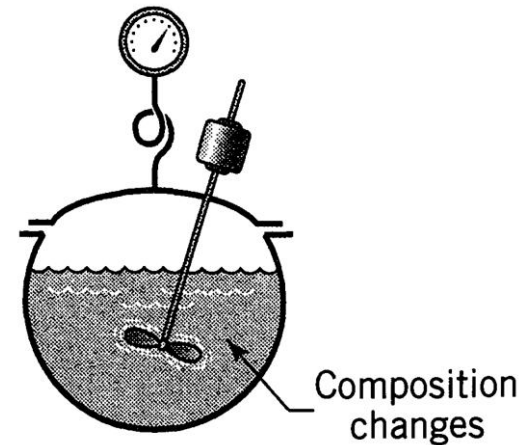


ESSENTIALS OF REACTOR DESIGN

- To arrive at a well fitted design:
 - we must be able to predict the response of the reacting system to changes in operating conditions (i.e. how rates and equilibrium conversion change with temperature and pressure),
 - we must be able to compare yields for alternative designs (adiabatic versus isothermal operations, single versus multiple reactor units, flow versus batch system), and
 - we must be able to estimate the economics of the various alternatives.

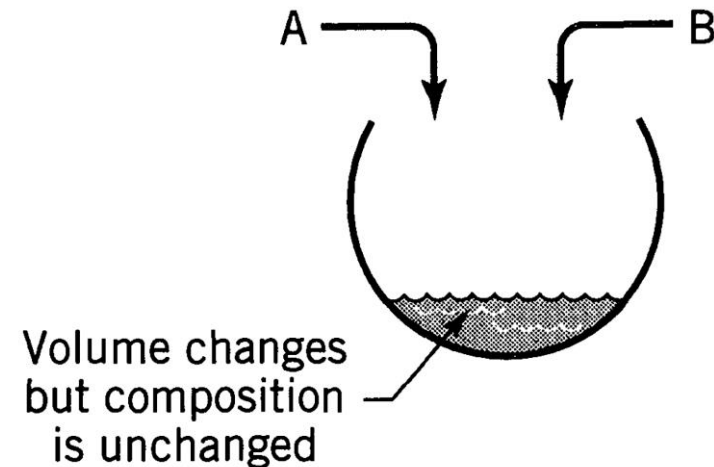
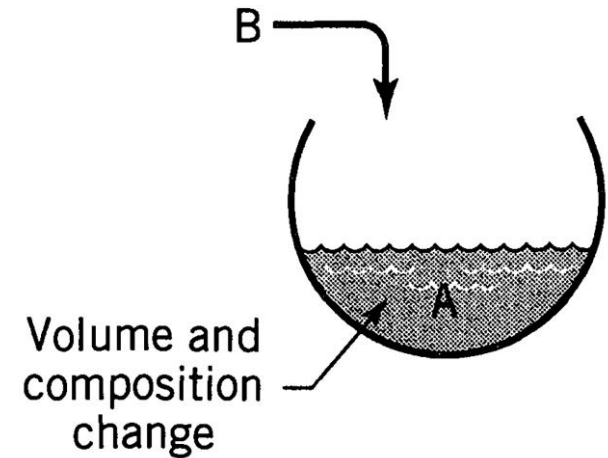
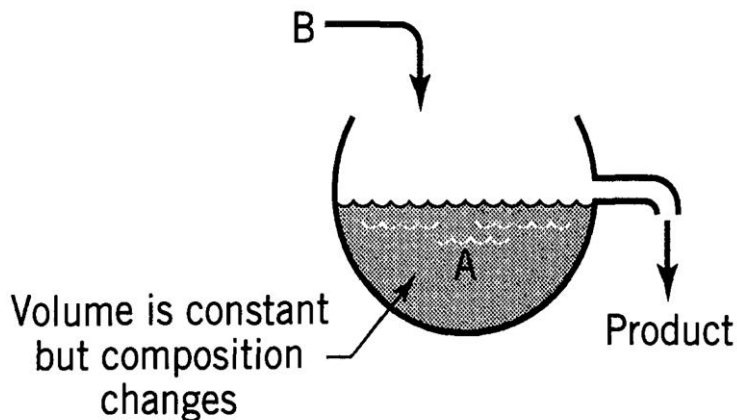
CLASSIFICATION OF REACTOR TYPES

- The batch reactor is
 - is used for small-scale experimental studies on reaction kinetics
 - used industrially when relatively small amounts of material are to be treated.
 - needs little supporting equipment
 - An ideal reactor
- The steady-state flow reactor is
 - used industrially when large quantities of material are to be processed
 - used when the rate of reaction is fairly high to extremely high
 - extremely good product quality control can be obtained
 - supporting equipment needs are great
 - widely used in the oil industry.



CLASSIFICATION OF REACTOR TYPES

- The semi-batch reactor
 - is a flexible system but is more difficult to analyze than the other reactor types
 - It offers good control of reaction speed because the reaction proceeds as reactants are added
 - Such reactors are used in a variety of applications from the calorimetric titrations in the laboratory to the large open hearth furnaces for steel production.

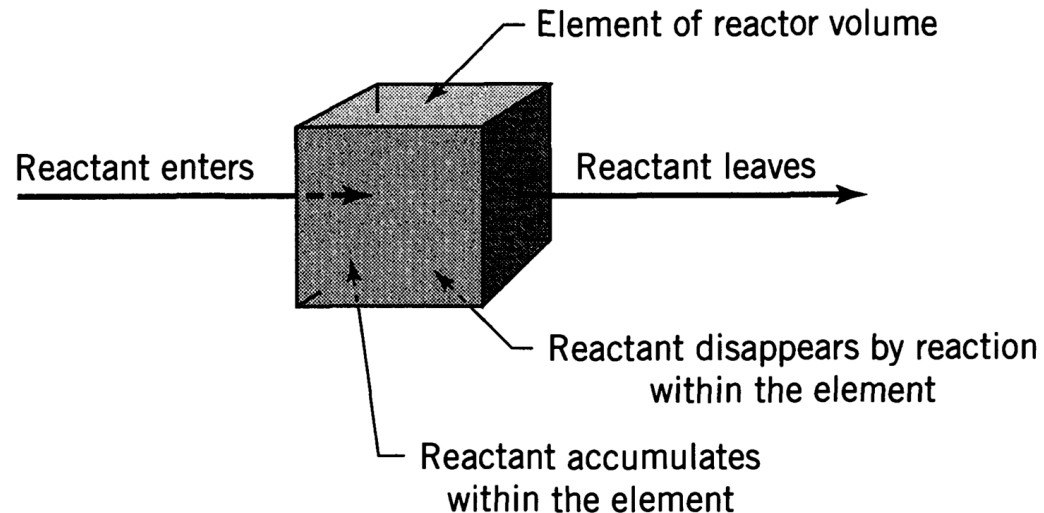


Comparison of Types of Chemical Reactors

Type of Reactor	Characteristics	Usage	Advantages	Disadvantages
Batch	<ul style="list-style-type: none"> Reactor is charged (filled) via two holes in the top of the tank; while reaction is carried out, nothing else is put in or taken out until reaction is done; tank easily cooled or heated by jacket 	<ul style="list-style-type: none"> Small-scale production Intermediate or one-shot productions Pharmaceuticals Fermentations 	<ul style="list-style-type: none"> High conversion per unit volume for one pass Same reactor can be used to produce one product one time and a different product the next 	<ul style="list-style-type: none"> High operating cost (labor) Product quality more variable than with continuous operation
Semibatch	<ul style="list-style-type: none"> Either one reactant is charged and the other is fed continuously (at small concentrations) or else one of the products can be removed continuously (to avoid side reactions) 	<ul style="list-style-type: none"> Small-scale production Competing reactions 	<ul style="list-style-type: none"> Good selectivity; feed can be controlled so as to minimize side runs. 	<ul style="list-style-type: none"> High operating labor cost Product quality more variable than with continuous operation
Continuously stirred tank reactor (CSTR)	<ul style="list-style-type: none"> Run at steady state with continuous flow of reactants and products; the feed assumes a uniform composition throughout the reactor, exit stream has the same composition as in the tank 	<ul style="list-style-type: none"> When agitation is required Series configuration for different concentration streams 	<ul style="list-style-type: none"> Continuous operation Good temperature control Good control Simplicity of construction Low operating (labor) cost 	<ul style="list-style-type: none"> Lowest conversion per unit volume Bypassing and channeling possible with poor agitation
Plug flow reactor (PFR)	<ul style="list-style-type: none"> Arranged as one long reactor or many short reactors in a tube bank; no radial variation in reaction rate (concentration); concentration changes with length down the reactor 	<ul style="list-style-type: none"> Large-scale production Homogeneous reactions Heterogeneous reactions Continuous production High temperature 	<ul style="list-style-type: none"> Highest conversion per unit volume Low operating labor cost Continuous operation Good heat transfer 	<ul style="list-style-type: none"> Undesired thermal gradients may exist Poor temperature control Shutdown, cleaning may be expensive
Tubular packed bed reactor (PBR)	<ul style="list-style-type: none"> Tubular reactor that is packed with solid catalyst particles 	<ul style="list-style-type: none"> Used primarily in heterogeneous gas phase reactions with a catalyst 	<ul style="list-style-type: none"> Highest conversion per unit mass of catalyst Low operating cost Continuous operation 	<ul style="list-style-type: none"> Undesired thermal gradients may exist Poor temperature control Channeling may occur

MATERIAL AND ENERGY BALANCES IN A REACTOR

- In any design process, the first thing to do is to carry out material and energy balances over the equipment to be designed.
- For the material balance, consider an element of volume of the reactor,



- The material balance for any reactant (or product) can be expressed as

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

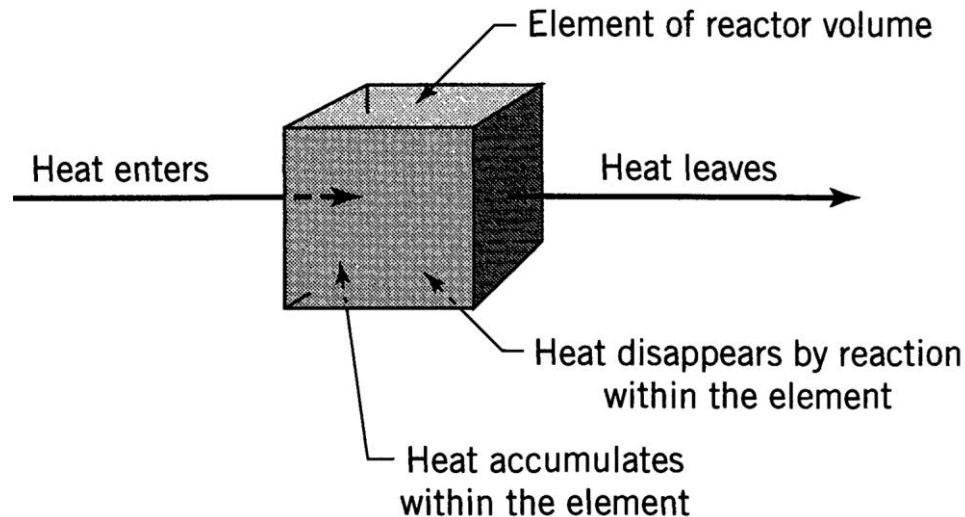


MATERIAL AND ENERGY BALANCES IN A REACTOR

- For constant composition within the reactor (i.e. independent of position),
 - the accounting is made over the whole reactor (synonymous to integral method).
- For variable composition,
 - the accounting must be made over a differential element of volume and then integrated across the whole reactor for the appropriate flow and concentration conditions (i.e. combining both the differential and integral method of analysis).
- For the various reactor types this material balance equation simplifies to the basic *performance equation* for that type of reactor.
 - in the batch reactor the first two terms are zero;
 - in the steady-state flow reactor the fourth term disappears;
 - in the semi-batch reactor all four terms may have to be considered.

ENERGY BALANCE IN A REACTOR

- In non-isothermal operations *energy balances* must be used in conjunction with material balances.
- Considering the element of volume of the reactor,



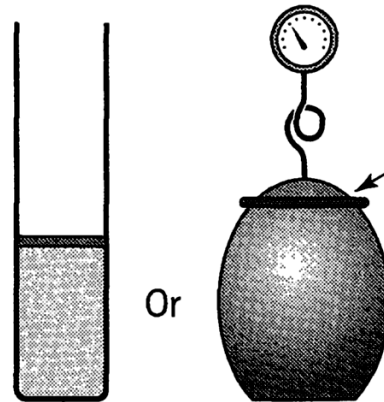
- The energy balance for any reactant (or product) is expressed as

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

SYMBOLS AND RELATIONSHIP BETWEEN C_A AND X_A

■ For a batch reactor,

At the start
 $t = 0$

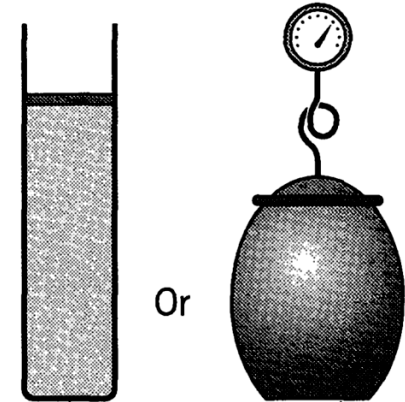


Constant pressure

Constant volume

Let time pass
~~~~~>

Later  
time =  $t$

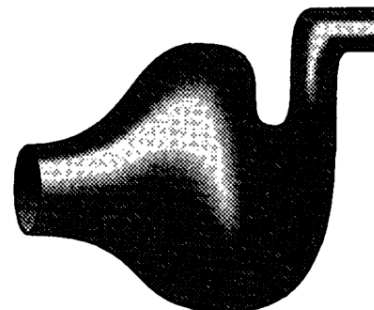


■ While for a steady state flow reactor,

$$\left. \begin{matrix} \pi_0 V_0 N_{A0} P_{A0} \\ C_{A0} X_{A0} = 0 \end{matrix} \right\}$$

$$\left. \begin{matrix} \pi V N_A P_A \\ C_A X_A \end{matrix} \right\}$$

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



$$\left. \begin{matrix} F_A = F_{A0}(1 - X_A) \\ v, C_A, X_A \end{matrix} \right\}$$

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

$V$  = volume



# SYMBOLS AND RELATIONSHIP BETWEEN $C_A$ AND $X_A$

- For the reaction:  $aA + bB \rightarrow rR$ .
- The previous figures show that there are two related measures of the extent of reaction, the concentration  $C_A$  and the conversion  $X_A$ .
- The relationship between  $C_A$  and  $X_A$  depends on a number of factors.
- Case 1. Constant Density Batch and Flow Systems.** It includes most liquid reactions and gas reactions run at constant temperature and density. Here  $C_A$  and  $X_A$  are related as follows:

$$\left. \begin{aligned} X_A &= 1 - \frac{C_A}{C_{A0}} \quad \text{and} \quad dX_A = -\frac{dC_A}{C_{A0}} \\ \frac{C_A}{C_{A0}} &= 1 - X_A \quad \text{and} \quad dC_A = -C_{A0}dX_A \end{aligned} \right\} \text{for } \varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}} = 0$$

- where  $\varepsilon_A$  is the fractional volume change on complete conversion of A, and

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



# SYMBOLS AND RELATIONSHIP BETWEEN $C_A$ AND $X_A$

- **Case 2. Batch and Flow Systems of Gases of Changing Density but with  $T$  and  $\pi$  Constant.** Here the density changes because of the change in number of moles during reaction. The volume of a fluid element changes linearly with conversion, or  $V = V_0 (1 + \varepsilon_A X_A)$

$$\left. \begin{aligned} X_A &= \frac{C_{A0} - C_A}{C_{A0} + \varepsilon_A C_A} & \text{and} & \quad dX_A = -\frac{C_{A0}(1 + \varepsilon_A)}{(C_{A0} + \varepsilon_A C_A)^2} dC_A \\ \frac{C_A}{C_{A0}} &= \frac{1 - X_A}{1 + \varepsilon_A X_A} & \text{and} & \quad \frac{dC_A}{C_{A0}} = -\frac{1 + \varepsilon_A}{(1 + \varepsilon_A X_A)^2} dX_A \end{aligned} \right\} \text{for } \varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}} \neq 0$$

- To follow changes in the other components we have

$$\text{between reactants } \begin{cases} \varepsilon_A X_A = \varepsilon_B X_B \\ \frac{a\varepsilon_A}{C_{A0}} = \frac{b\varepsilon_B}{C_{B0}} \end{cases} \quad \text{for products and inerts } \begin{cases} \frac{C_R}{C_{A0}} = \frac{(r/a)X_A + C_{R0}/C_{A0}}{1 + \varepsilon_A X_A} \\ \frac{C_I}{C_{I0}} = \frac{1}{1 + \varepsilon_A X_A} \end{cases}$$



# SYMBOLS AND RELATIONSHIP BETWEEN $C_A$ AND $X_A$

- Case 3. Batch and Flow Systems for Gases in General (varying  $p, T, \pi$ ) which react according to



- Selecting a key reactant, A as the basis for determining the conversion, then for ideal gas behavior,

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

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

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



# SYMBOLS AND RELATIONSHIP BETWEEN $C_A$ AND $X_A$

- For high-pressure non-ideal gas behavior replace

$$\left(\frac{T_0\pi}{\tau_0\pi_0}\right) \text{ by } \left(\frac{z_0T_0\pi}{zT\pi}\right)$$

where  $z$  is the compressibility factor.

- To change to another key reactant, say B, note that

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

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

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

# SYMBOLS AND RELATIONSHIP BETWEEN $C_A$ AND $X_A$

## Example 1:

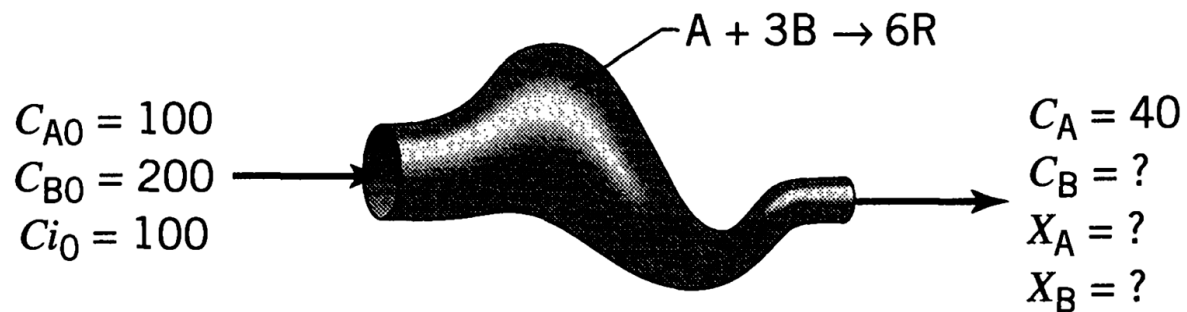
Consider a feed  $C_{A0} = 100$ ,  $C_{B0} = 200$ ,  $C_{i0} = 100$  to a steady-flow reactor. The isothermal gas-phase reaction is



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

## SOLUTION:

- First sketch what is known



- Next recognize that this problem concerns [Case 2](#).
- So evaluate  $\varepsilon_A$  and  $\varepsilon_B$ .





# SYMBOLS AND RELATIONSHIP BETWEEN $C_A$ AND $X_A$

- Remember  $\varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}}$  and  $\varepsilon_B = \frac{\varepsilon_A C_{B0}}{b C_{A0}}$

- Let's take volumes of entering gas to be 400

$$\text{at } X_A = 0 \quad V = 100A + 200B + 100i = 400$$

$$\text{at } X_A = 1 \quad V = 0A - 100B + 600R + 100i = 600$$

- So

$$\varepsilon_A = \frac{600 - 400}{400} = \frac{1}{2}$$

- And

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

- Therefore, calculating for  $X_A$ ,

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



# SYMBOLS AND RELATIONSHIP BETWEEN $C_A$ AND $X_A$

- Calculating for  $X_B$ ,

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

- And calculating for  $C_B$ ,

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



**THANK YOU  
FOR  
YOUR  
ATTENTION!  
ANY QUESTIONS?**



# SYMBOLS AND RELATIONSHIP BETWEEN $C_A$ AND $X_A$

- **Case 2. Batch and Flow Systems of Gases of Changing Density but with  $T$  and  $\pi$  Constant.** Here the density changes because of the change in number of moles during reaction. The volume of a fluid element changes linearly with conversion, or  $V = V_0 (1 + \varepsilon_A X_A)$

$$\left. \begin{aligned} X_A &= \frac{C_{A0} - C_A}{C_{A0} + \varepsilon_A C_A} & \text{and} & \quad dX_A = -\frac{C_{A0}(1 + \varepsilon_A)}{(C_{A0} + \varepsilon_A C_A)^2} dC_A \\ \frac{C_A}{C_{A0}} &= \frac{1 - X_A}{1 + \varepsilon_A X_A} & \text{and} & \quad \frac{dC_A}{C_{A0}} = -\frac{1 + \varepsilon_A}{(1 + \varepsilon_A X_A)^2} dX_A \end{aligned} \right\} \text{for } \varepsilon_A = \frac{V_{X_A=1} - V_{X_A=0}}{V_{X_A=0}} \neq 0$$

- To follow changes in the other components we have

$$\begin{array}{l} \text{between} \\ \text{reactants} \end{array} \left\{ \begin{array}{l} \varepsilon_A X_A = \varepsilon_B X_B \\ \frac{a\varepsilon_A}{C_{A0}} = \frac{b\varepsilon_B}{C_{B0}} \end{array} \right. \quad \begin{array}{l} \text{for products} \\ \text{and inerts} \end{array} \left\{ \begin{array}{l} \frac{C_R}{C_{A0}} = \frac{(r/a)X_A + C_{R0}/C_{A0}}{1 + \varepsilon_A X_A} \\ \frac{C_I}{C_{I0}} = \frac{1}{1 + \varepsilon_A X_A} \end{array} \right.$$

