

**Chemical Reaction Engineering I**  
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**Lecture 06**  
**Stoichiometry for Variable Volume Flow System**

Welcome to the third lecture of module 3 of Chemical Reaction Engineering I. In this module we are discussing Stoichiometry. Before going to this lecture let us have brief recap on our previous lecture.

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**Recap**

**Topics covered in previous lecture**

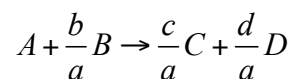
- Stoichiometry for constant volume flow system
- Stoichiometry for variable volume batch system

$$v = v_0 \quad C_A = \left( \frac{F_{A0}}{v} \right) (1-X) = C_{A0} (1-X) \quad 1 + \frac{b}{a} X \rightarrow \frac{c}{a} + \frac{d}{a} X$$

$$\theta_B = \frac{F_B}{F_A} \quad C_B = C_{A0} \left( \theta_B - \frac{b}{a} X \right) \rightarrow \text{so on.}$$

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

In our previous lecture we have broadly covered this two topics, one is stoichiometry for constant volume flow system, and second topic we have covered the stoichiometry for variable volume batch system. In case of stoichiometry for constant volume flow system, we have seen when v volumetric flow rate v is equal to v<sub>0</sub> for a general reactions,



For this general reaction we have seen how the concentration C<sub>A</sub> is related with the conversion. That means

$$C_A = \frac{F_A}{v} = \frac{F_{A0}(1-X)}{v}$$

X is the conversion. So this is essentially  $C_{A0} = \frac{F_{A0}}{v_0}$  that is the initial concentration that is  $C_{A0}(1 - X)$ .

Similarly, for component B

$$C_B = C_{A0} \left( \Theta_B - \left( \frac{b}{a} \right) X \right)$$

and so on. In this case this  $\Theta_B$  is nothing but

$$\Theta_B = \frac{F_B}{F_A}$$

For stoichiometry for variable volume batch system we have obtained the relations between volume and the conversion. So the volume for case of batch reactor is V is related with the conversion as

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

So this is the general expression for variable volume batch system where the volume is related with the conversion. And then we can relate with the concentration.

Here, if we incorporate constant volume systems we will essentially get the constant volume batch reactor equation.

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## Module 2: Lecture 3

### Stoichiometry for Variable Volume Flow System

#### Lecture Outline

- Stoichiometry for variable volume flow system ✓
- Summary on stoichiometry ✓

Now in this lecture, we will consider stoichiometry for variable volume flow system and the lecture outline would be, stoichiometry for variable volume flow system, and then we will summarize stoichiometry whatever discussed till today.

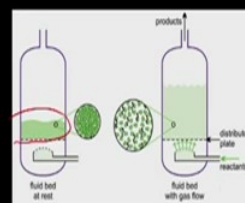
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### Stoichiometry in Variable Volume Flow System

The expression for variable volume flow can be obtained similar way to the variable volume batch system.



Some examples



So, let us start with stoichiometry in variable volume flow system. The expression for variable volume flow system would be similar to that of the variable volume batch system. In a similar way we can obtain the stoichiometry table. Some examples of variable volume flow systems are you can see the cooking gas cylinder as you can see with fitted regulator. So if you just open the regulator the flow will start and the volume will change. So it is the volume gradually decrease inside the reactor inside this cylinder.

Other examples for variable volume flow systems like if we have fluidized bed at rest and then we pass you can see the fluidized bed how it looks like at rest. Now, if we pass the reactant to pass through the bed through the distributor so the bed will expand. So essentially the volume of this will change so this is another examples of variable volume flow system.

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**Stoichiometry in Variable Volume Flow System**

**What we want?**

$v = f(X)$

**Total concentration at any point in the reactor:**  $C_T = \frac{P}{ZRT}$

**At reactor entrance:**  $C_{T0} = \frac{P_0}{Z_0RT_0}$

**We know for flow system:**  $C_T = \frac{F_T}{v} \Rightarrow F_T = C_T v$  ✓

$C_{T0} = \frac{F_{T0}}{v_0} \Rightarrow F_{T0} = C_{T0} v_0$  ✓

Now, what we want for this? We want volumetric flow rate small  $v$  would be in terms of the function of conversion. The total concentration at any point in the reactor we can write

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

Where  $P$  is the pressure and  $Z$  as defined earlier for the batch system it is the compressibility factor,  $R$  is the universal gas constant and  $T$  is the temperature. So the total concentration at any point in the reactor we can write

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

Now the same concentration at the reactor entrance, what would be the equation? At reactor entrance we can write at  $t = 0$ .

So the pressure of the system we can consider

$$C_{T0} = \frac{P_0}{Z_0RT_0}$$

$T_0$  is the initial temperature and  $Z_0$  is the compressibility factor at the reactor entrance and  $R$  is the universal gas constant.

Now, we know for any flow system the concentration  $C_T$  can be related with the molar flow rate by the volumetric flow rate. So  $C_T$  can be written as

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

So from here we can write

$$F_T = C_T v$$

Now for  $C_{T0}$  we can write

$$C_{T0} = \frac{F_{T0}}{v_0}$$

$C_{T0}$  is the concentration at the volumetric flow rate at the reactor entrance and from here we can write

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

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**Stoichiometry in Variable Volume Flow System**

Total concentration at any point in the reactor:  $C_T = \frac{P}{ZRT}$

At reactor entrance:  $C_{T0} = \frac{P_0}{Z_0 R T_0}$

We know for flow system:  $C_T = \frac{F_T}{v} \Rightarrow F_T = C_T v$

$C_{T0} = \frac{F_{T0}}{v_0} \Rightarrow F_{T0} = C_{T0} v_0$

$F_T = C_T v = \frac{P}{ZRT} v$        $F_{T0} = C_{T0} v_0 = \frac{P_0}{Z_0 R T_0} v_0$

Divide and considering  $Z = Z_0$ :  $v = v_0 \left( \frac{F_T}{F_{T0}} \right) \left( \frac{P_0}{P} \right) \left( \frac{T_0}{T} \right) \times \left( \frac{Z_0}{Z} \right) \rightarrow 1$

Now this we know, if we just write  $F_T$  would be

$$F_T = C_T \nu$$

So  $C_{T0}$  as we said at the entrance conditions. At the total concentration at any point in the reactant  $C_T$  so this will be  $\frac{P_0}{Z_0 RT_0}$  so if we substitute  $C_T$  in place of here so this  $F_T$  we can write  $\frac{P}{ZRT} \nu$ . Similarly for  $F_{T0}$  we can write  $C_{T0} \nu_0$  and  $C_{T0}$  we know from here so we can substitute this over here and we will get

$$F_{T0} = \frac{P_0}{Z_0 RT_0} \nu_0$$

Now, if we divide these two relations,

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

$$F_{T0} = C_{T0} \nu_0 = \frac{P_0}{Z_0 RT_0} \nu_0$$

this one and one and we would obtain this relation. So basically, we divide

$$\frac{\frac{P}{ZRT} \nu}{\frac{P_0}{Z_0 RT_0} \nu_0} = \frac{F_T}{F_{T0}}$$

So if we rearrange this we would obtain  $\nu$  would be

$$\nu = \nu_0 \left( \frac{F_T}{F_{T0}} \right) \left( \frac{P_0}{P} \right) \left( \frac{T}{T_0} \right) \left( \frac{Z}{Z_0} \right)$$

So if we considered  $Z$ , the compressibility factor  $Z$  would not change much at the reactor entrance and at the any point in the reactor so this we can take as 1.

$$\frac{Z}{Z_0} = 1$$

So in that case we would obtain this relation.

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

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**Stoichiometry in Variable Volume Flow System**

Devide and considering  $Z = Z_0$ :  $v = v_0 \left(\frac{F_T}{F_{T0}}\right) \frac{P_0}{P} \left(\frac{T}{T_0}\right)$

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

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

$\varepsilon = y_{A0} \delta$

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

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

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

Now we have this relation and we know  $F_T$  is related with the stoichiometry of the reactions as

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

So, if we substitute  $F_T$  in this relation we would obtain  $v$  would be

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

So this equation we would obtain.

Now, if we just rearrange this relation we can write as

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

Earlier we have discussed that

$$\frac{F_{A0}}{F_{T0}} = y_{A0}$$

so we can write

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



Now as from the definition of the  $\varepsilon$  we have obtained that this is equal to  $y_{A0}\delta$ , so if we substitute here we will obtain

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

So finally this is the relation which will get with the conversion and extend of reaction with the volumetric flow rate.

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**Stoichiometry in Variable Volume Flow System**

**Express**       $C = f(X)$

**Concentration of any species j for a flow system in terms of conversion:**

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

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

**For component A:**       $C_A = F_A/v = C_{T0} \frac{F_A}{F_T} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$

**For component B:**       $C_B = C_{T0} \left(\frac{F_B}{F_T}\right) \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$

Now our target is to express the concentration in terms of the function of X. So we got the relations between the volumetric flow rate and the conversion now our target is to express the concentration in terms of the conversion. So concentration of any species j for a flow system in terms of the conversion we can write

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

Since

$$C_{T0} = \frac{F_{T0}}{v_0}$$

so we can substitute over here Cj would be

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

So here this expression of concentration is for any component j.

Now if we write for component A, this relation would be

$$C_A = \frac{F_A}{v} = C_{T0} \left(\frac{F_A}{F_T}\right) \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$$

So this is equations of  $C_A$ . Similarly, we can write for component B we can write  $C_B$  would be

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

So we have relation of CB as well.

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**Stoichiometry in Variable Volume Flow System**

**Express**  $C = f(X)$

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

**Concentration of any species j for a flow system in terms of conversion:**  $C_j = \frac{F_j}{v} = \frac{F_j}{v_0 (1 + \varepsilon X) \left(\frac{P_0}{P}\right) \left(\frac{T}{T_0}\right)} = \frac{F_j}{v_0 (1 + \varepsilon X)} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$

**For component A:**  $C_A = \frac{F_{A0}(1-X)}{v_0 (1 + \varepsilon X)} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right) = C_{A0} \frac{(1-X)}{(1 + \varepsilon X)} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$

**For component B:**  $C_B = \frac{F_B}{v} = \frac{F_{A0} \left(\Theta_B - \frac{b}{a} X\right)}{v_0 (1 + \varepsilon X)} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right) = \frac{C_{A0} \left(\Theta_B - \frac{b}{a} X\right)}{(1 + \varepsilon X)} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$

Now,

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

This we have, we have derived this relation. Now for any component j we have this relation

$$C_j = \frac{F_j}{v}$$

If we substitute this relation of v in this expression of in place of v we would get

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

Now to simplify it would be

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

So this is the relation of  $C_j$ .

Now, we can write for component A which would be

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

and if we simplify

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

So now similarly for component B we can write  $C_B$  would be

$$C_B = \frac{F_B}{\nu} = \frac{F_{A0}}{\nu_0} \left(\Theta_B - \left(\frac{b}{a}\right)X\right)$$

And we have defined the  $\Theta$  earlier, so

$$C_B = C_{A0} \frac{\left(\Theta_B - \left(\frac{b}{a}\right)X\right)}{(1+\epsilon X)} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$$

So this is the relations where we can relate concentration with the conversion.

Now from this we can develop the stoichiometric table for the flow system which can be written as follows flow and particularly gas flow system the stoichiometric table for the first 4 column that species, their no change of concentration, and then remaining those columns remains same in the case of the constant volume flow system. And it will be similar to the variable volume flow system. But the conversion term between the concentration and the flow rate would be little different so which will summarize in this stoichiometric table.

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**Stoichiometric Table in Variable Volume Gas Flow System**

$$C_A = \frac{F_A}{\nu} = \frac{F_{A0}(1-X)}{\nu_0(1+\epsilon X)} = \frac{F_{A0}(1-X)}{\nu_0} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$$

$$C_B = \frac{F_B}{\nu} = \frac{F_{A0}\left(\Theta_B - \frac{b}{a}X\right)}{\nu_0(1+\epsilon X)} = \frac{F_{A0}\left(\Theta_B - \frac{b}{a}X\right)}{\nu_0} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$$

$$C_C = \frac{F_C}{\nu} = \frac{F_{A0}\left(\Theta_C + \frac{c}{a}X\right)}{\nu_0(1+\epsilon X)} = \frac{F_{A0}\left(\Theta_C + \frac{c}{a}X\right)}{\nu_0} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$$

$$C_D = \frac{F_D}{\nu} = \frac{F_{A0}\left(\Theta_D + \frac{d}{a}X\right)}{\nu_0(1+\epsilon X)} = \frac{F_{A0}\left(\Theta_D + \frac{d}{a}X\right)}{\nu_0} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$$

$$C_I = \frac{F_I}{\nu} = \frac{F_{A0}\Theta_I}{\nu_0(1+\epsilon X)} = \frac{F_{A0}\Theta_I}{\nu_0} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$$

So we can write  $C_A$

$$C_A = \frac{F_A}{\nu} = \frac{F_{A0}(1-X)}{\nu} = \frac{F_{A0}(1-X)}{\nu_0(1+\varepsilon X)} \left(\frac{T_0}{T}\right) \left(\frac{P}{P_0}\right) = C_{A0} \frac{(1-X)}{(1+\varepsilon X)} \left(\frac{T_0}{T}\right) \left(\frac{P}{P_0}\right)$$

For  $C_B$  we can write

$$C_B = \frac{F_B}{\nu} = \frac{F_{A0}(\Theta_B - (\frac{b}{a})X)}{\nu} = \frac{F_{A0}(\Theta_B - (\frac{b}{a})X)}{\nu_0(1+\varepsilon X)} \left(\frac{T_0}{T}\right) \left(\frac{P}{P_0}\right) = C_{A0} \frac{(\Theta_B - (\frac{b}{a})X)}{(1+\varepsilon X)} \left(\frac{T_0}{T}\right) \left(\frac{P}{P_0}\right)$$

For  $C_C$  we can write

$$C_C = \frac{F_C}{\nu} = \frac{F_{A0}(\Theta_C + (\frac{c}{a})X)}{\nu} = \frac{F_{A0}(\Theta_C + (\frac{c}{a})X)}{\nu_0(1+\varepsilon X)} \left(\frac{T_0}{T}\right) \left(\frac{P}{P_0}\right) = C_{A0} \frac{(\Theta_C + (\frac{c}{a})X)}{(1+\varepsilon X)} \left(\frac{T_0}{T}\right) \left(\frac{P}{P_0}\right)$$

Similarly for  $C_D$

$$C_D = \frac{F_D}{\nu} = \frac{F_{A0}(\Theta_D + (\frac{d}{a})X)}{\nu} = \frac{F_{A0}(\Theta_D + (\frac{d}{a})X)}{\nu_0(1+\varepsilon X)} \left(\frac{T_0}{T}\right) \left(\frac{P}{P_0}\right) = C_{A0} \frac{(\Theta_D + (\frac{d}{a})X)}{(1+\varepsilon X)} \left(\frac{T_0}{T}\right) \left(\frac{P}{P_0}\right)$$

And for inert we can write

$$C_I = \frac{F_I}{\nu} = \frac{F_{A0}\Theta_I}{\nu} = \frac{F_{A0}\Theta_I}{\nu_0(1+\varepsilon X)} \left(\frac{T_0}{T}\right) \left(\frac{P}{P_0}\right) = \frac{C_{A0}\Theta_I}{(1+\varepsilon X)} \left(\frac{T_0}{T}\right) \left(\frac{P}{P_0}\right)$$

So this is the conversion of different concentration in terms of conversion and the extent of reaction.

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### Stoichiometry in Flow System: Example

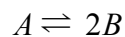
Consider the following elementary reaction with equilibrium constant,  $K=50$  L/mol and initial reactant concentration,  $C_{A0}=0.5$  mol/L.



$$-r_A = k_A \left[ C_A - \frac{C_B^2}{K} \right]$$

Find the equilibrium conversion,  $X_{ef}$  for a flow reactor

Now, let us take an example considered the same example which we have covered in case of the constant volume batch reactor. So consider also the variable volume batch reactor. So consider the following elementary reactions with equilibrium constant,  $K = 50$  liter per mole and initial reactant concentration is  $C_{A0} = 0.5$  mole per litre. So this is the reaction



which is a reversible reaction and rate of reaction is given

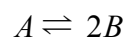
$$-r_A = k_A \left[ C_A - \frac{C_B^2}{K} \right]$$

Find the equilibrium conversion  $X_{ef}$  for a flow reactor.

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Stoichiometry in Flow System: Example				
Find the equilibrium conversion, $X_{ef}$ for a flow reactor				
Symbol	Initial	Change	Remaining	
A	$F_{A0}$	$-F_{A0}X$	$F_A = F_{A0}(1-X)$	$A \rightarrow 2B$
B	0	$+F_{A0}X/2$	$F_B = F_{A0}X/2$	
Totals: $F_{T0} = F_{A0}$		$F_T = F_{A0} + F_{A0}X$		

So we have to find out the conversion  $X_{ef}$  for a flow reactor where



Now, we can develop the stoichiometry table like symbol A for component A, the initial concentration is  $F_{A0}$ , the change is  $-F_{A0}X$  so the remaining  $F_A$  would be equal to  $F_{A0}(1-X)$ .

Now for component B, initial concentration of component B is zero and its change would be

$$+\frac{F_{A0}X}{2}, \text{ so } F_B \text{ would be } \frac{F_{A0}X}{2}.$$

Now  $F_{T0}$  would be  $F_{A0}$  initially and  $F_T$  would be  $F_{A0} + F_{A0}X$

So if we sum up this two we will get

$$F_T = F_{A0} + F_{A0}X$$

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## Stoichiometry in Flow System: Example

Isothermal  $T=T_0$

Isobaric  $P=P_0$

$$v = v_0(1 + \varepsilon X)$$

$$C_A = \frac{F_{A0}(1-X)}{v_0(1+\varepsilon X)} = \frac{C_{A0}(1-X)}{(1+\varepsilon X)}$$

$$C_B = \frac{F_{A0}2X}{v_0(1+\varepsilon X)} = \frac{2C_{A0}(1-X)}{(1+\varepsilon X)}$$

Now the system is isothermal  $T$  is equal to  $T_0$  and the isobaric system that is  $P$  is equal to  $P_0$ .

So in this case  $v$  would be equal to

$$v = v_0(1 + \varepsilon X)$$

And  $C_A$  would be

$$C_A = \frac{F_{A0}(1-X)}{v_0(1+\varepsilon X)}$$

So since this is isobaric and isothermal system the ratio between the temperature and the pressure they are unity. They are 1 so they are cancelled out. So we will have  $C_A$  would be

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

We know the initial concentration which are given  $\varepsilon$  also we can calculate so we will get the relations between concentration and conversion.

Similarly for component B we can write

$$C_B = \frac{F_{A0}2X}{v_0(1+\varepsilon X)}$$

So if we substitute over here we will get

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

So we obtained the relations for  $C_A$  and  $C_B$  in terms of the conversion from the stoichiometry table.

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**Stoichiometry in Flow System: Example**

$$-r_A = k_A \left[ C_A - \frac{C_B^2}{K} \right]$$

$$-r_A = k_A \left[ \left( \frac{C_{A0}(1-X_f)}{(1+\varepsilon X_f)} \right) - \left( \frac{2C_{A0}X_f}{(1+\varepsilon X_f)K} \right)^2 \right]$$

Pure A  $\rightarrow y_{A0}=1, C_{A0}=y_{A0}P_0/RT_0, C_{A0}=P_0/RT_0$

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

At equilibrium:  $-r_A=0$

$$K^2(1-X_{ef}) = \frac{4C_{A0}X_{ef}^2}{(1+\varepsilon X_{ef})} \Rightarrow \frac{X_{ef}^2}{(1+\varepsilon X_{ef})(1-X_{ef})} = \frac{K^2}{4C_{A0}}$$

Now, this is the rate expression and if we substitute  $C_A$  and  $C_B$  which we have developed in the relations earlier, we can write

$$r_A = C_A C_{A0} (1 - X_f)$$

Here  $X_f$  represents the conversion in flow system. In batch system we have written  $X$ , in flow system we change to  $X_f$ , so  $X_f$  is the conversion in the flow system. So we can write

$$-r_A = k_A \left[ \left( \frac{C_{A0}(1-X_f)}{(1+\varepsilon X_f)} \right) - \left( \frac{2C_{A0}X_f}{(1+\varepsilon X_f)K} \right)^2 \right]$$

So pure component A we will have

$$y_{A0} = 1$$

$$C_{A0} = \frac{y_{A0}P_0}{RT_0}$$

Since  $y_{A0} = 1$ , so from here we can write

$$C_{A0} = \frac{P_0}{RT_0}$$

Here  $y_{A0} = 1$ , so we substitute it here 1

In case of  $\varepsilon$  and  $\delta$  we can see

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

2 minus 1, 2 moles is fo

So in this case if we substitute that part we would have

$$K^2(1 - X_{ef}) = \frac{4C_{A0}X_{ef}^2}{(1 + \varepsilon X_{ef})}$$

$X_{ef}$  is the equilibrium conversion. So, if we solve it we will get now this relation,

$$\Rightarrow \frac{X_{ef}^2}{(1 + \varepsilon X_{ef})(1 - X_{ef})} = \frac{K^2}{4C_{A0}}$$

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**Stoichiometry in Flow System: Example**

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

$$\frac{X_{ef}^2}{(1 + \varepsilon X_{ef})(1 - X_{ef})} = \frac{K^2}{4C_{A0}}$$

$$\Rightarrow \frac{X_{ef}^2}{(1 + X_{ef})(1 - X_{ef})} = \frac{50 \times 50}{4 \times 0.5} = 1250$$

$$\Rightarrow \frac{X_{ef}^2}{(1 - X_{ef}^2)} = 1250 \Rightarrow X_{ef}^2 = 1250 - 1250X_{ef}^2$$

$$\Rightarrow 1251X_{ef}^2 = 1250 \Rightarrow X_{ef} = \pm \sqrt{\frac{1250}{1251}} = \pm 0.9996$$

$X_{ef} = 0.9996$

$X_{ef} = 0.963$

So now,  $\varepsilon$  would be

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

we have calculated and this is the equation which we have derived.

$$\Rightarrow \frac{X_{ef}^2}{(1 + \varepsilon X_{ef})(1 - X_{ef})} = \frac{K^2}{4C_{A0}}$$

Now, if we substitute the values here K is 50 which is given and initial concentration is 0.5

$$\Rightarrow \frac{X_{ef}^2}{(1 + \varepsilon X_{ef})(1 - X_{ef})} = \frac{50 * 50}{4 * 0.5} = 1250$$

So if we solve it, it would be

$$\frac{X_{ef}^2}{(1 - X_{ef}^2)} = 1250$$

$$X_{ef}^2 = 1250 - 1250X_{ef}^2$$

Now, if we rearrange we can get

$$1251X_{ef}^2 = 1250$$

and from here we can write  $X_{ef}$  would be equal to

$$X_{ef} = \pm \sqrt{\frac{1250}{1251}} = \pm 0.9996$$

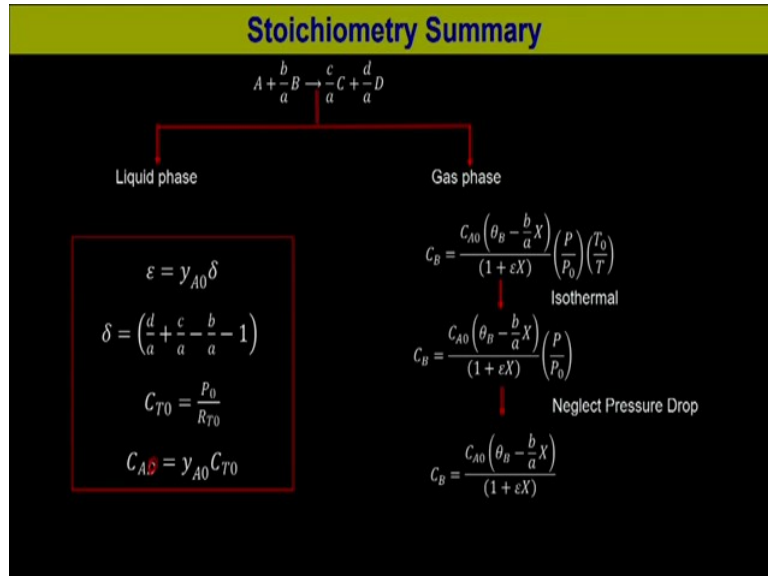
So if we take the square root of this it would be

$$X_{ef} = \pm 0.9996$$

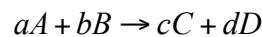
So the equilibrium conversion in this case we can write  $X_{ef} = 0.9996$  because the conversion cannot be the negative so we will take the positive root so which is 0.9996.

Now, if we recall our earlier solutions for the batch reactor flow systems. In that case for the same example we obtained the equilibrium conversion as  $X_e$  is 0.963. So it could see the conversion for this case is higher than the conversion compared to the batch reactor conversion.

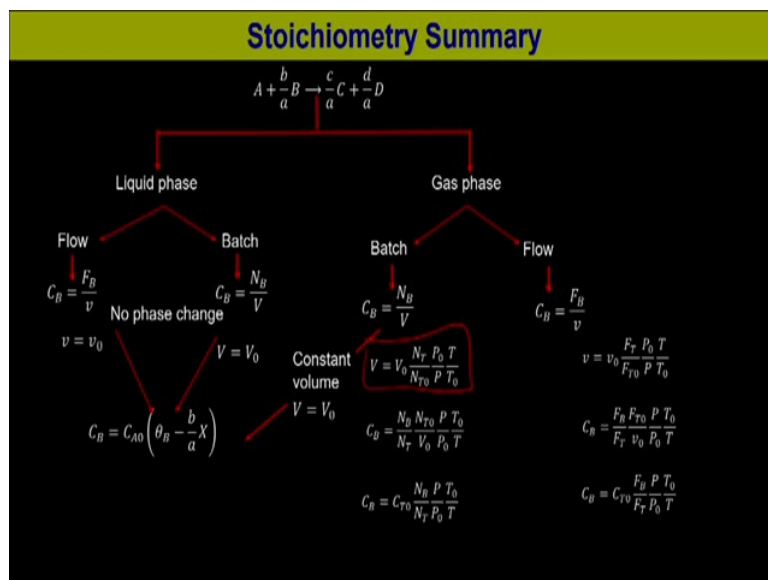
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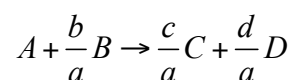
Now, let us summarize what we have discussed so far in the stoichiometry. So we have considered the general relations of component A and B they reacts and they form product C and D with a stoichiometric coefficient a for component A, stoichiometric coefficient b for component B and producing C of C stoichiometric coefficient c and D with stoichiometric coefficient c that means



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And we have considered A is the limiting reactants so we have considered



So this is the overall general reactions we have considered. And then we have considered liquid phase and gas phase both the reactions. Reactions occurred in the liquid phase and reaction occurred in the gas phase. Now flow system and batch system we have considered,

for flow system we can write  $C_B = \frac{F_B}{\nu}$  and for batch system we can write  $C_B = \frac{N_B}{V}$ . So

capital V is the volume of the reactor. Now in the gas phase batch reactor  $C_B = \frac{N_B}{V}$  and for

flow reactor we have also it will be similar to the liquid phase  $C_B = \frac{F_B}{\nu}$ .

Now if there is no phase change in the system. Suppose in the liquid phase there is no phase change so  $\nu = \nu_0$ . And in this case the volumetric flow rate would be  $\nu_0$  constant. And in this case batch reactor they does not change much the volume does not change much, so we can keep  $V = V_0$ . The volume will remain as constant. So we can write

$$C_B = C_{A0} \left( \Theta_B - \left( \frac{b}{a} \right) X \right)$$

In case of gas phase if the constant volume system  $V = V_0$  then we can write

$$V = V_0 \left( \frac{N_T}{N_{T0}} \right) \left( \frac{P_0}{P} \right) \left( \frac{T}{T_0} \right)$$

This is for variable volume system. Similarly, for variable volume flow systems we can write

$$\nu = \nu_0 \left( \frac{F_T}{F_{T0}} \right) \left( \frac{P_0}{P} \right) \left( \frac{T}{T_0} \right)$$

Similarly,

$$C_B = \frac{N_B}{N_T} \left( \frac{F_B}{V_0} \right) \left( \frac{P}{P_0} \right) \left( \frac{T_0}{T} \right)$$

that is for batch reactor.

In case of flow reactor we can write

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

And so we can write, this rearrange this relations

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

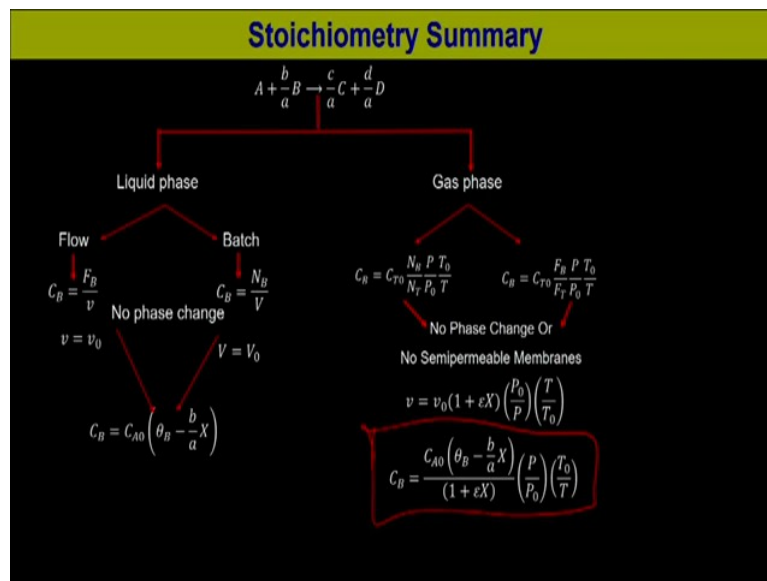
Similarly, in case of the flow reactor we can write

$$C_B = C_{T0} \frac{N_B}{N_T} \left( \frac{P}{P_0} \right) \left( \frac{T_0}{T} \right)$$

But if it is constant volume, batch reactor  $V = V_0$  so in that case we will obtain this relation even if in the gas phase.

$$C_B = C_{A0} \left( \Theta_B - \left( \frac{b}{a} \right) X \right)$$

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Now, if there is no phase change or no semipermeable membrane in this case for gas phase. Both batch and the flow reactor we can write

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

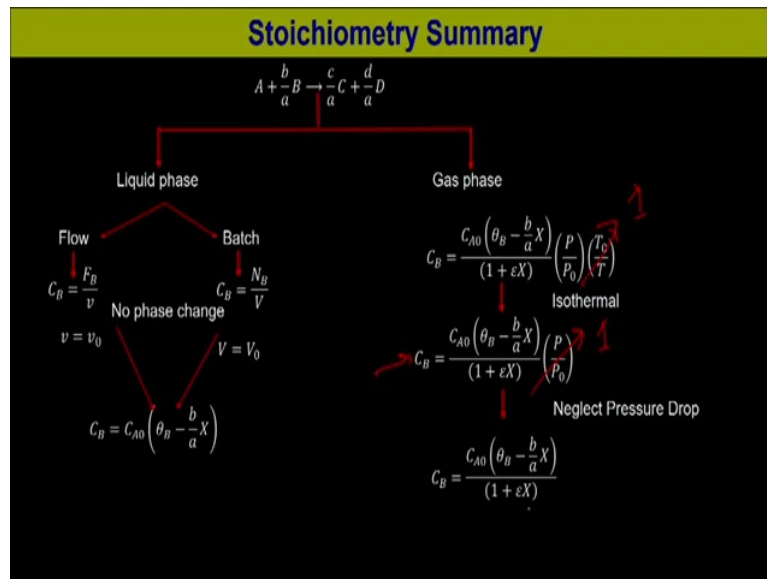
and CB we can write

$$C_B = C_{A0} \frac{\left( \Theta_B - \frac{b}{a}X \right)}{(1 + \epsilon X)} \left( \frac{P}{P_0} \right) \left( \frac{T_0}{T} \right)$$

So this is how we can obtain for the gas phase system where there is no phase change.

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If it is isothermal then  $\frac{T_0}{T} = 1$  so we will get

$C_B$  would be like this

$$C_B = C_{A0} \frac{\left( \Theta_B - \left( \frac{b}{a} \right) X \right)}{(1 + \epsilon X)} \left( \frac{P}{P_0} \right)$$

If it is isobaric stem that is neglect pressure drop isobaric system then  $\frac{P}{P_0} = 1$ .

So finally we will get

$$C_B = C_{A0} \frac{\left( \Theta_B - \left( \frac{b}{a} \right) X \right)}{(1 + \epsilon X)}$$

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**Stoichiometry Summary**

$$A + \frac{b}{a}B \rightarrow \frac{c}{a}C + \frac{d}{a}D$$

Liquid phase

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

$$\delta = \left(\frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1\right)$$

$$C_{T0} = \frac{P_0}{RT_0}$$

$$C_{A0}\delta = y_{A0}C_{T0}$$

Gas phase

$$C_B = \frac{C_{A0} \left(\theta_B - \frac{b}{a}X\right)}{(1 + \varepsilon X)} \left(\frac{P}{P_0}\right) \left(\frac{T_0}{T}\right)$$

↓ Isothermal

$$C_B = \frac{C_{A0} \left(\theta_B - \frac{b}{a}X\right)}{(1 + \varepsilon X)} \left(\frac{P}{P_0}\right)$$

↓ Neglect Pressure Drop

$$C_B = \frac{C_{A0} \left(\theta_B - \frac{b}{a}X\right)}{(1 + \varepsilon X)}$$

And  $\delta$  we have now  $\varepsilon$  we have obtained earlier  $\varepsilon = y_{A0}\delta$  and  $\delta$  is the change in mole into the reacting systems that is

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

And

$$C_{T0} = \frac{P_0}{RT_0}$$

And

$$C_{A0}\delta = C_{A0} = y_{A0}C_{T0}$$

So this is the overall summary of the stoichiometry chapter which we have discussed in 3 lectures. And this would be the basis for solving the other reactor design part in other sections which we will cover in other modules. So thank you very much for attending this lecture and we will continue our discussion on the other modules in the next lecture.