Chemical Reaction Engineering I
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Lecture 05
Stoichiometry for Constant Volume Flow and Variable Volume Batch Systems

Welcome to the second lecture of module 2 of Chemical Reaction Engineering 1. In this module we are discussing Stoichiometry. So before going to this lecture let us brief recap on our previous lecture.

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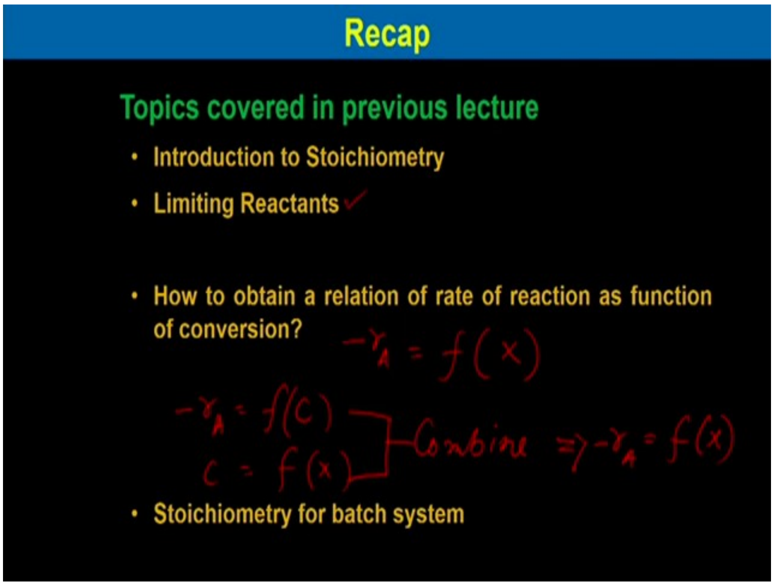

Recap

Topics covered in previous lecture

- Introduction to Stoichiometry
- Limiting Reactants ✓
- How to obtain a relation of rate of reaction as function of conversion? $-r_A = f(x)$

$$\left.\begin{array}{l} -r_A = f(C) \\ C = f(x) \end{array}\right] \text{Combine} \Rightarrow -r_A = f(x)$$

- Stoichiometry for batch system

The topic which we have discussed in our previous lecture is the introduction to Stoichiometry and we have discussed why this Stoichiometry is important for chemical reaction engineering. For any conversion between the concentration to the extent of reactions or the relations between the rate of reactions with the concentrations can be related with the help of Stoichiometry and this in turn will help us to design the chemical reactor.

The second thing which we have discussed is the limiting reactants. Suppose in the reaction you will have more than one reactants then which reactants will limit the extent of reaction has to be considered. So it depends on the Stoichiometry and the Stoichiometry of the reactants reacting into the system and the concentration of the reactants initially present. So this we have discussed with an example.

The next thing which we have considered how to obtain a relation of rate of reactions as function of conversion? Here we need to know the rate $-r_A$ is function of conversion.

$$-r_A = f(X)$$

So to do that what we need to know? We know the rate of reactions $-r_A$ as a function of concentration of the component.

$$-r_A = f(C)$$

And from Stoichiometry we know the relations between concentrations as a function of conversion.

$$C = f(X)$$

So, if we combine these 2 then we will obtain in the relations between rate of reactions as a function of conversion. Then we have discussed the Stoichiometry for a batch system and we have considered the constant volume batch system.

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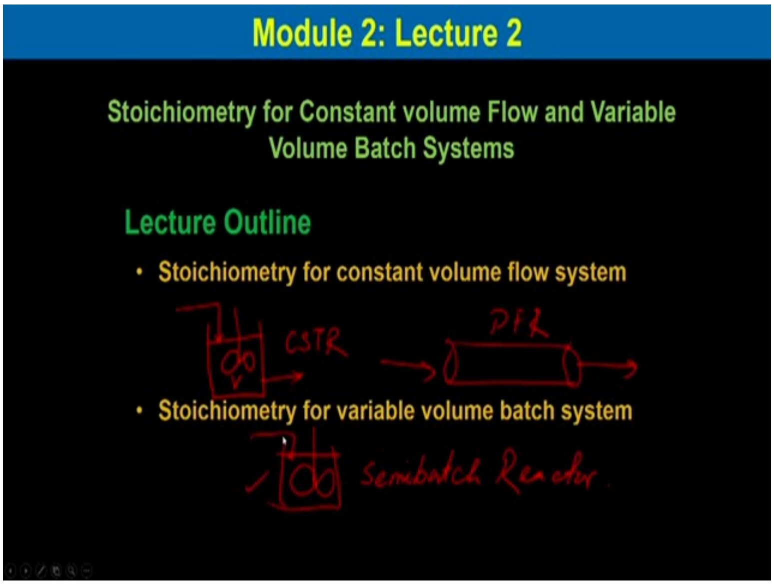

Module 2: Lecture 2

Stoichiometry for Constant volume Flow and Variable Volume Batch Systems

Lecture Outline

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

In this lecture, we will consider Stoichiometry for constant volume flow and variable volume batch systems. The lecture outline are Stoichiometry for constant volume flow systems that means we have two different kind of flow systems as we have considered is two ideal reactors, one is CSTR that is continuous stirred tank reactor. So the reactant is fed and the product is out. So this is continuous process and we call CSTR.

And the volume V over here is a constant, we will consider at the beginning. And then another type of ideal reactor is the plug flow reactor. So this flow reactors we will consider how to relate for Stoichiometry for the flow systems. And also we will consider Stoichiometry for variable volume batch systems. That means if we take a reactor, batch reactor and it is closed and for constant volume batch reactor what we do, we used to take the reactants and then close it and do the reactions and take out the product and we consider the volume of the reactants does not change after the chemical reactions.

But it may so happen that the total moles of the system may before the chemical reactions and after the chemical reactions may change and in turn it will change the volume of the systems or if we consider the semi-batch systems where you have a continuous flow in to the reactant in, into the reactor and there is no outlet, so which we call the semi-batch reactor. So in this case we would see there is change in volume. So these 2 things we will consider.

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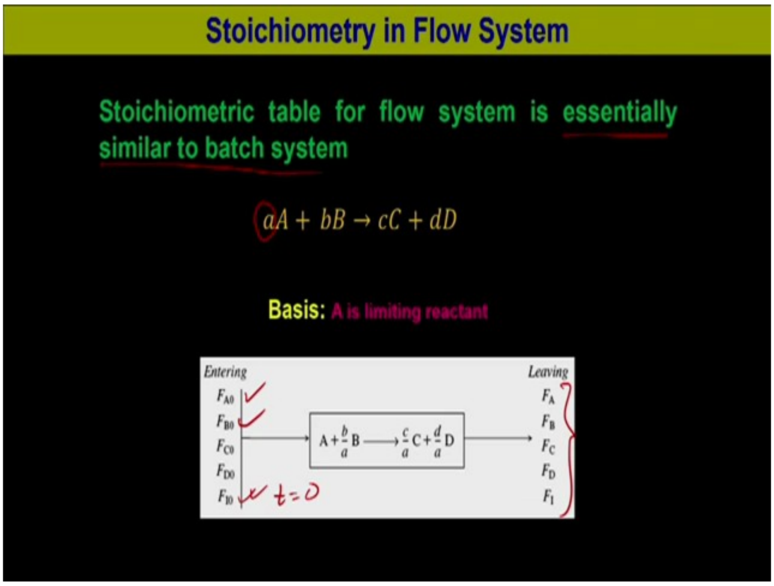

Stoichiometry in Flow System

Stoichiometric table for flow system is essentially similar to batch system

$$aA + bB \rightarrow cC + dD$$

Basis: A is limiting reactant

So let us consider Stoichiometry in flow systems. The Stoichiometry table for flow system is essentially similar to the batch systems, but in this case there is a flow in and flow out continuously into the system, so it is a flow system. The Stoichiometry table would be almost similar like the batch system. Now, let us consider general reactions

$$aA + bB \rightarrow cC + dD$$

That means a moles of reactant A reacts with b mole of B producing c mole of C and d mole of D.

So, in this case what would be the limiting reactant we have to consider as a basis? So if we consider A as a basis then the Stoichiometry coefficient of the reactants in the reactions may be divided throughout the all the species. So essentially you will get,

$$A+\frac{b}{a}B$$

So if we divide this A that is the limiting reactants throughout this all the reactants and products, so you will have the coefficient 1 for A

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

Now, if you consider a flow reactor like this and you reactant which are entering into the reactor is F_{A0} is the concentration or the molar flow rate of component A and F_{B0} is the molar flow rate of component B. F_{C0} is the molar flow rate of component C. F_{D0} is the molar flow rate of component D and F_{I0} is the molar flow rate of component I, so this naught represents at the entering conditions maybe at t equal to 0.

And as you can see from the chemical reaction A and B is reacting, so F_A and F_B they are reactants, F_C and F_D they are the products and I as the inert, so the leaving flow rate after the chemical reactions is considered as F_A for component A, F_B for component B, F_C for component C, F_D for component D and F_I for component I, so these are the leaving conditions.

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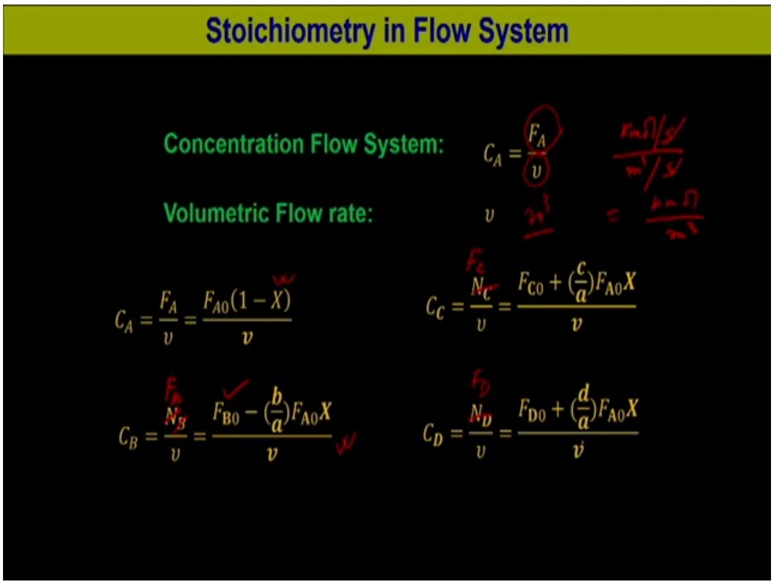

Stoichiometry in Flow System

Concentration Flow System: $C_A = \frac{F_A}{v}$ $\frac{\cancel{kmol/s}}{m^3/\cancel{s}}$

Volumetric Flow rate: v $\underline{m^3}$ $= \frac{kmol}{m^3}$

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

$$C_C = \frac{\overset{F_C}{\cancel{N_C}}}{v} = \frac{F_{C0} + (\frac{c}{a})F_{A0}X}{v}$$

$$C_B = \frac{\overset{F_B}{\cancel{N_B}}}{v} = \frac{F_{B0} - (\frac{b}{a})F_{A0}X}{v}$$

$$C_D = \frac{\overset{F_D}{\cancel{N_D}}}{v} = \frac{F_{D0} + (\frac{d}{a})F_{A0}X}{v}$$

Now, if you consider a flow system, its concentration C_A can be defined is the molar flow rate by the volumetric flow rate. So as F_A if we consider mole or kilo mole its units we can write kilo mole per time second divided by the volumetric flow rate v is the meter cube per second. So this will cancel out, so essentially you will get the unit of concentration is kilo mole per meter cube. So this is the concentration definition for the flow system.

Now, the volumetric flow rate as we said is v and having unit of meter cube per second. So CA would be

$$C_A = \frac{F_A}{v}$$

which would be equal to if there is conversion of the component A is defined as X. So then F_A we can write

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

So then we can write

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

Similarly, for component B this would be

$$C_B = \frac{F_B}{v} = \frac{F_{B0} - (\frac{b}{a})F_{A0}X}{v}$$

So, if we look into the chemical reactions that is

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

So one mole of a reacts with $\frac{b}{a}$ moles of B, so then your concentration initially was F_{B0} and B by a $F_{A0}X$ is reacted because the conversion is X and for one mole of A $F_{A0}X$ is the concentration which is reacted, so for $\frac{b}{a}$ moles B will react, $(\frac{b}{a})F_{A0}X$ as we have discussed earlier for constant volume batch reactor. Similar way it would be

$$\frac{F_{B0} - (\frac{b}{a})F_{A0}X}{v}$$

So this is concentration B we can define this way,

$$C_B = \frac{F_{B0} - (\frac{b}{a})F_{A0}X}{v}$$

Now concentration of C, so this would be

$$C_C = \frac{F_C}{v}$$

so this would be

$$C_C = \frac{F_{C0} + (\frac{c}{a})F_{A0}X}{v}$$

because C is the component which is product.

Similarly for D this would be

$$C_D = \frac{F_D}{v}$$

so it would be

$$C_D = \frac{F_D}{v} = \frac{F_{D0} + (\frac{d}{a})F_{A0}X}{v}$$

So we can represent the concentration for flow systems using the molar flow rate and the volumetric flow rate of the components.

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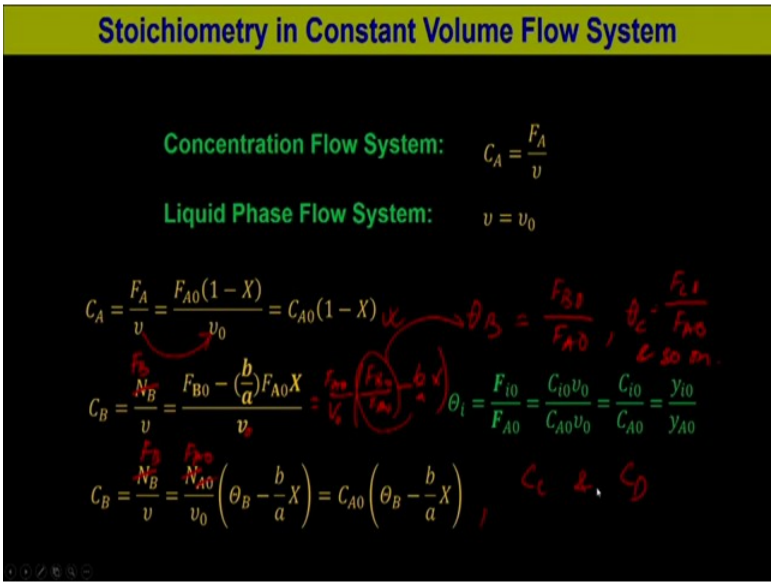

Stoichiometry in Constant Volume Flow System

Concentration Flow System: $C_A = \frac{F_A}{v}$

Liquid Phase Flow System: $v = v_0$

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

$$C_B = \frac{\overset{F_B}{\cancel{N_B}}}{v} = \frac{F_{B0} - (\frac{b}{a})F_{A0}X}{v_0} = \frac{F_{A0}}{v_0}\left(\frac{F_{B0}}{F_{A0}} - \frac{b}{a}X\right)$$

$$\theta_i = \frac{F_{i0}}{F_{A0}} = \frac{C_{i0}v_0}{C_{A0}v_0} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}}$$

$$\theta_B = \frac{F_{B0}}{F_{A0}}, \quad \theta_C = \frac{F_{C0}}{F_{A0}}$$ & so on.

$$C_B = \frac{\overset{F_B}{\cancel{N_B}}}{v} = \frac{\overset{F_{A0}}{\cancel{N_{A0}}}}{v_0}\left(\theta_B - \frac{b}{a}X\right) = C_{A0}\left(\theta_B - \frac{b}{a}X\right)$$

C_C & C_D

Now, concentration as we said

$$C_A = \frac{F_A}{v}$$

and if we consider liquid phase system in general for liquids phase systems the volumetric flow rate does not change much. In most of the cases for the gas phase reactions the volumetric flow rate change. So if it so happened for liquid phase system we can assume $v = v_0$ which is constant. In that case we can replace for this concentration terms which is

$$\frac{F_A}{v} = \frac{F_{A0}(1-X)}{v_0}$$

So we replace v with v_0.

So then from the definition we can write

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

then it would be

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

Similarly, for B we can write

$$\frac{\frac{F_B}{v}}{} = \frac{F_{B0} - (\frac{b}{a})F_{A0}X}{v_0}$$

As you know we can define Θ for any component I as

$$\Theta_i = \frac{F_{i0}}{F_{A0}} = \frac{C_{i0}v_0}{C_{A0}v_0} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}}$$

So for component B, if we put this relation Θ_B would be

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

Similarly, for Θ_C it would be

$$\Theta_C = \frac{F_{C0}}{F_{A0}}, \text{ and so on.}$$

So now, if we use this relations over here we can write $\frac{F_B}{v}$ would be

$$\frac{F_{B0} - (\frac{b}{a})F_{A0}X}{v_0}$$

If we just take F_{A0} outside the bracket, so this would be F_{B0}, so you can write over here,

$$\frac{F_{A0}}{v_0}(\frac{F_{B0}}{F_{A0}} - (\frac{b}{a})X)$$

So this would be $\frac{F_{A0}}{v_0}$ into this term we will replace with Θ_B.

So

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

Similar way we can write for C_C and C_D.

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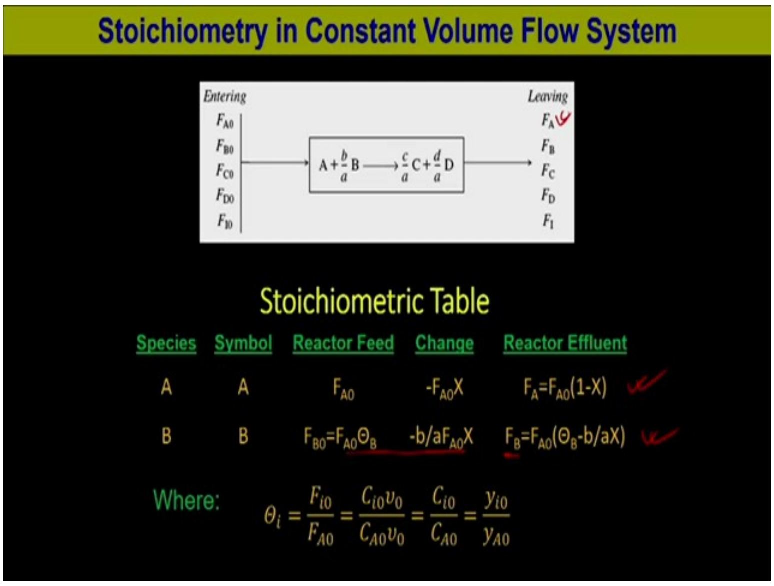

Stoichiometry in Constant Volume Flow System

Stoichiometric Table

Species	Symbol	Reactor Feed	Change	Reactor Effluent
A	A	F_{A0}	$-F_{A0}X$	$F_A=F_{A0}(1-X)$
B	B	$F_{B0}=F_{A0}\Theta_B$	$-b/aF_{A0}X$	$F_B=F_{A0}(\Theta_B-b/aX)$

Where: $\theta_i = \frac{F_{i0}}{F_{A0}} = \frac{C_{i0}v_0}{C_{A0}v_0} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}}$

Now this is our systems, where we have entering molar flow rates and this is the exiting molar flow rates, so in this case if we wanted to develop the stoichiometric table, so we can write the species that means A, B, C, D and I these are the species and the symbol which we use then the reactor feed and then the change in the concentration or change in their moles then the reactor effluents.

So for component A, species A we used symbol A and feed to the reactor is F_{A0}, so the change which happened due to the chemical reactions is $F_{A0}X$ and the affluent which we get F_A would be equal to $F_{A0}(1-X)$. So this is, means initially we had one mole and $F_{A0}X$ is reacted, so initially we had F_{A0} mole and $F_{A0}X$ is reacted, so

$$F_A = F_{A0} - F_{A0}X$$

would be

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

which is the affluent here.

Now for component B, as we have seen that it is represented with symbol B, so

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

and the change in the reactions which would happen is

$$-(\frac{b}{a})F_{A0}X$$

so this is the change due to the reactions with A. So then the remaining affluent would be

$$F_{A0}(\Theta_B - (\frac{b}{a})X)$$

Then from these 2 we can write

$$F_B = F_{A0}(\Theta_B - (\frac{b}{a})X)$$

So this is the reactor affluent. So here Θ_i as we have discussed earlier is $\frac{F_{i0}}{F_{A0}}$, so based on that the Θ_B is represented over here.

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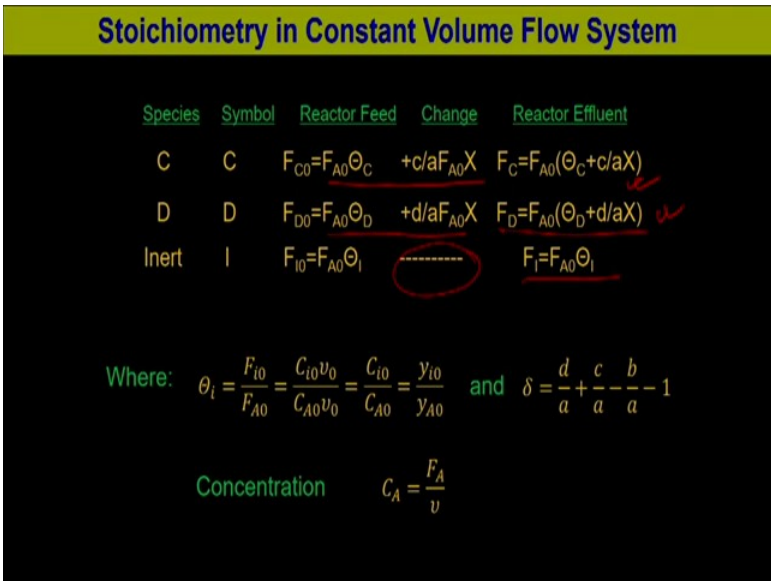

Stoichiometry in Constant Volume Flow System

Species	Symbol	Reactor Feed	Change	Reactor Effluent
C	C	$F_{C0}=F_{A0}\Theta_C$	$+c/aF_{A0}X$	$F_C=F_{A0}(\Theta_C+c/aX)$
D	D	$F_{D0}=F_{A0}\Theta_D$	$+d/aF_{A0}X$	$F_D=F_{A0}(\Theta_D+d/aX)$
Inert	I	$F_{I0}=F_{A0}\Theta_I$	---------	$F_I=F_{A0}\Theta_I$

Where: $\theta_i = \frac{F_{i0}}{F_{A0}} = \frac{C_{i0}\upsilon_0}{C_{A0}\upsilon_0} = \frac{C_{i0}}{C_{A0}} = \frac{y_{i0}}{y_{A0}}$ and $\delta = \frac{d}{a} + \frac{c}{a} - \frac{b}{a} - 1$

Concentration $C_A = \frac{F_A}{\upsilon}$

Now for other 2 components the products C is the species and symbol is used C this is a product. So F_{C0} is the reactor feed which is equal to $F_{A0}\Theta_C$ and the change that means the product which you will produce is $+(\frac{c}{a})X$. So the change would happen, would be equal to

$$F_C = F_{A0}(\Theta_C + (\frac{c}{a})X)$$

And we can also write for D in a similar way because it is the product $\frac{d}{a}$ mole of D is produced. So from this we can write

$$F_D = F_{A0}(\Theta_D + (\frac{d}{a})X)$$

Now we have inert into the system which does not react. So initially we had F_{I0} is the inert feed to the reactions, so F_{I0} would be $F_{A0}\Theta_I$ in this case there will be no change due to the chemical reactions because this is incorporated as an inert species. So there will not be any change of the feed and the outlet conditions or affluent conditions. So F_I would be equal to $F_{A0}\Theta_I$. So similar way Θ_I can be represented by $\frac{F_{I0}}{F_{A0}}$ over here.

Now, the change in the total mole because of the chemical reactions we can write is δ that is

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

this is the total change of the moles into the system and the concentration is

$$C_A = \frac{F_A}{\nu}$$

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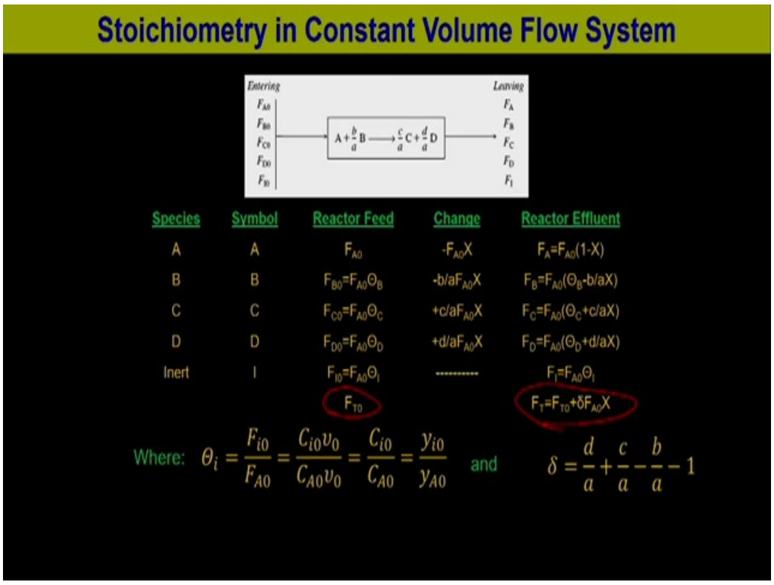

Stoichiometry in Constant Volume Flow System

Species	Symbol	Reactor Feed	Change	Reactor Effluent
A	A	F_{A0}	$-F_{A0}X$	$F_A=F_{A0}(1-X)$
B	B	$F_{B0}=F_{A0}\Theta_B$	$-b/aF_{A0}X$	$F_B=F_{A0}(\Theta_B-b/aX)$
C	C	$F_{C0}=F_{A0}\Theta_C$	$+c/aF_{A0}X$	$F_C=F_{A0}(\Theta_C+c/aX)$
D	D	$F_{D0}=F_{A0}\Theta_D$	$+d/aF_{A0}X$	$F_D=F_{A0}(\Theta_D+d/aX)$
Inert	I	$F_{I0}=F_{A0}\Theta_I$	----------	$F_I=F_{A0}\Theta_I$
		F_{T0}		$F_T=F_{T0}+\delta F_{A0}X$

Where: $\theta_i=\frac{F_{i0}}{F_{A0}}=\frac{C_{i0}v_0}{C_{A0}v_0}=\frac{C_{i0}}{C_{A0}}=\frac{y_{i0}}{y_{A0}}$ and $\delta=\frac{d}{a}+\frac{c}{a}-\frac{b}{a}-1$

So finally this is the overall stoichiometric table where we have represented all the species feed to the reactor and the change which would happen inside the reactors and the affluent which is coming out. Now if we sum of the reactor feed that would be F_{T0}, so we can sum of all the feeds and the affluent which is coming out is F_T. So if we sum of them it would be

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

The Delta is nothing but,

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

So this is the total feed and this is at inlet and this is at outlet conditions or living conditions. So this way we can obtain the stoichiometric table for a flow system.

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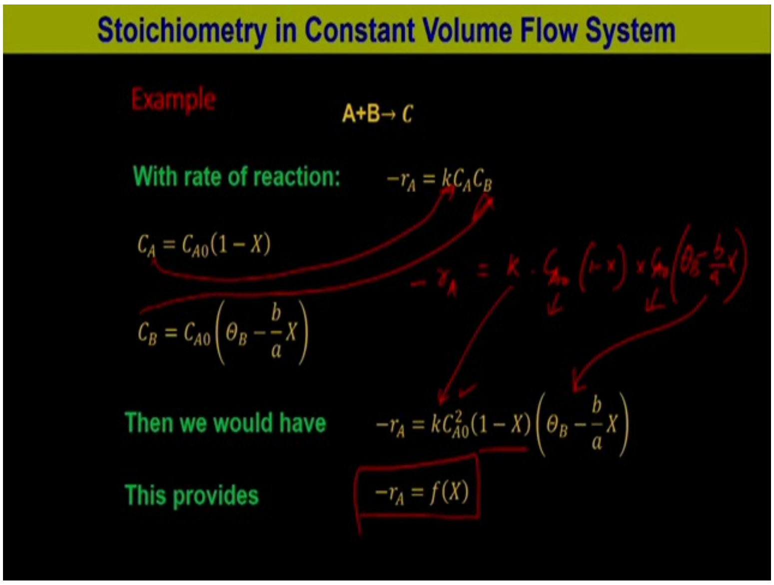

Stoichiometry in Constant Volume Flow System

Example $A+B \rightarrow C$

With rate of reaction: $-r_A = kC_AC_B$

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

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

$-r_A = k \cdot C_{A0}(1-X) \times C_{A0}\left(\theta_B - \frac{b}{a}X\right)$

Then we would have $-r_A = kC_{A0}^2(1-X)\left(\theta_B - \frac{b}{a}X\right)$

This provides $\boxed{-r_A = f(X)}$

Now, if we take an example say

$$A + B \rightarrow C$$

with the rate of reaction is given

$$-r_A = kC_AC_B$$

second order reactions and

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

and

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

then we would have $-r_A$ would be equal to we will replace this C_A over $-r_A$ and C_B over $-r_A$. So if we replace over here, so it would be C_{A0}, so basically

$$-r_A = k\ C_{A0}(1-X)\ C_{A0}(\Theta_B - (\frac{b}{a})X)$$

Now this would be

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

So we will get the relations between rate of reaction with the conversion. So this provides the rate of reactions as a function of conversion. Basically the concentration term will be replaced with the conversion term and then you will get the relations between rate of reactions with the conversion.

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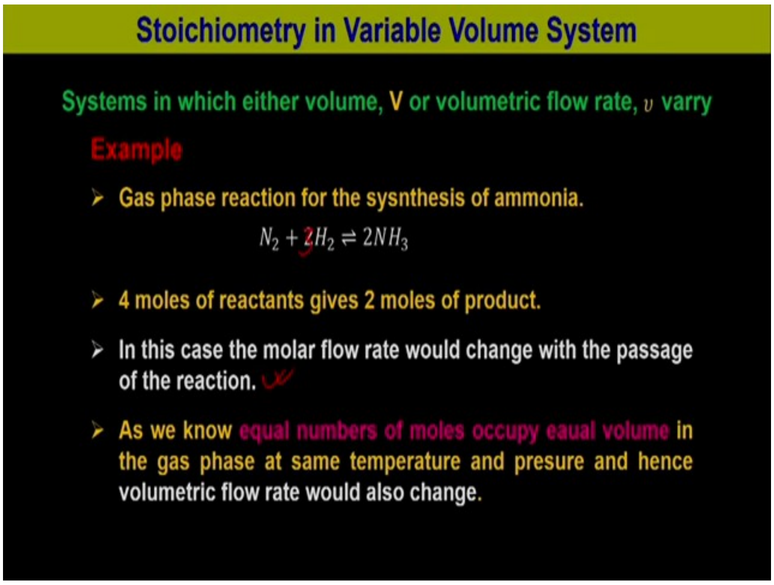

Stoichiometry in Variable Volume System

Systems in which either volume, V or volumetric flow rate, υ varry

Example

- Gas phase reaction for the sysnthesis of ammonia.

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$

- 4 moles of reactants gives 2 moles of product.
- In this case the molar flow rate would change with the passage of the reaction.
- As we know equal numbers of moles occupy eaual volume in the gas phase at same temperature and presure and hence volumetric flow rate would also change.

Now system in which either volume or the volumetric flow rate ν vary, so in that case we cannot treat the systems either flow or the constant volume systems either flow or the batch systems as a no constant volume system because the volumes of the reactor or the volumetric flow rate they are changing.

For example, the gas phase reactions for the synthesis of ammonia. We know the well-known reactions of ammonia productions the Haber process where we know Nitrogen is reacted with hydrogen and it forms ammonia. So this is

$$N_2 + 3H_2 \rightleftharpoons 2NH_3$$

So as we can see 4 moles, 1 mole of nitrogen and 3 mole of hydrogen that reacts and gives the product 2 moles. So during this gas phase reactions the total moles changes from 4 moles to the 2 mole product. In this case the molar flow rate would change with the passage of the reaction.

Now as we know equal number of moles occupy equal volume in gas phase at the same temperature and pressure and hence volumetric flow rate would also change. So in this case because of the change in the total moles as a reaction progress the volumetric flow rate would also change because as we know the equal moles occupy equal volume at a particular temperature and pressure. So this is one of the example of variable volume system.

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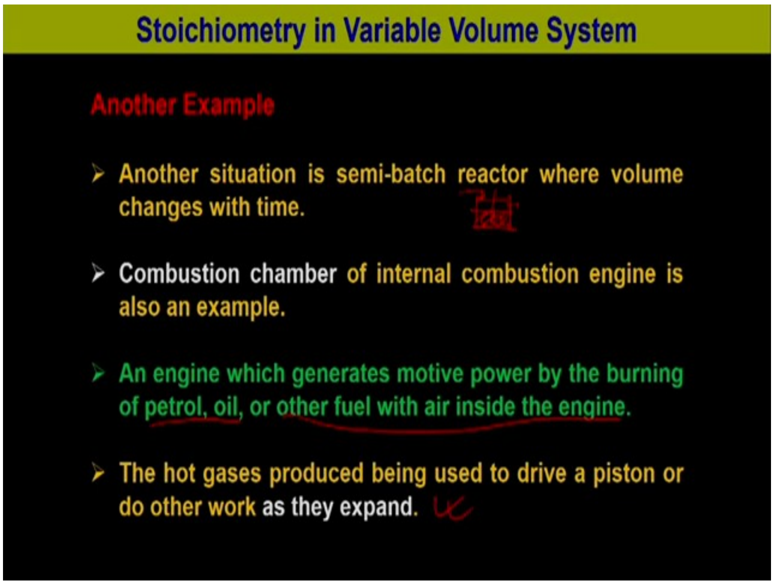

Stoichiometry in Variable Volume System

Another Example

- Another situation is semi-batch reactor where volume changes with time.
- Combustion chamber of internal combustion engine is also an example.
- An engine which generates motive power by the burning of petrol, oil, or other fuel with air inside the engine.
- The hot gases produced being used to drive a piston or do other work as they expand.

Another example is the semi-batch reactor where the volume changes with time. So basically in this case if we take as we have said earlier, you take a small amount of reactant initially and disclose and you have impeller, now you just slowly feed another reactant into it, so that A and B they are reacting, so if it is batch reactor and you are continuously stirring and you are adding certain component reactant into it. So the volume will essentially change from time to time. So this is one of another example of variable volume system.

Combustion chamber of internal combustion engine is also an example of variable volume system. An engine which generates motive power by burning petrol, oil or other fuel with air inside an engine that also changes the volume. The hot gases produced being used to drive a piston or do other work as they expand those are also examples of variable volume systems. So if the volume changes either it is batch reactor or it is flow reactors, if the volume changes how we can relate the conversion with the change in volume.

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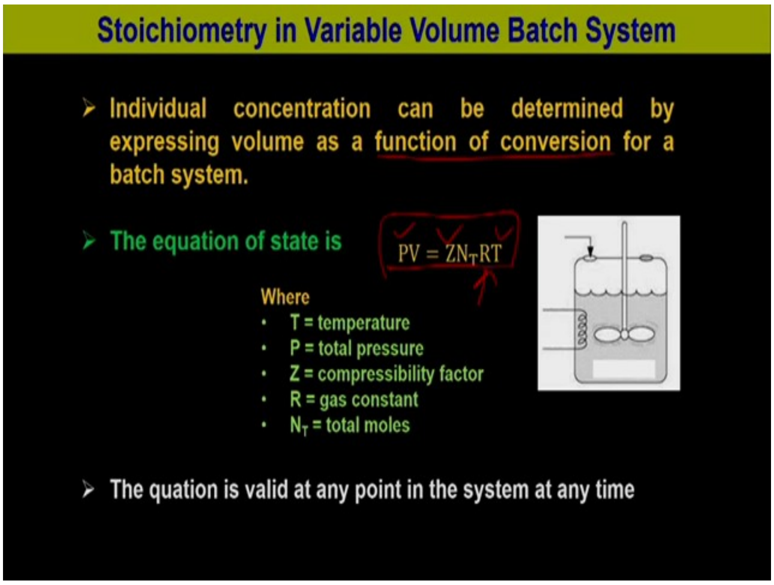

Stoichiometry in Variable Volume Batch System

- Individual concentration can be determined by expressing volume as a function of conversion for a batch system.
- The equation of state is $PV = ZN_TRT$

Where
- T = temperature
- P = total pressure
- Z = compressibility factor
- R = gas constant
- N_T = total moles

- The quation is valid at any point in the system at any time

Now, let us consider Stoichiometry in variable volume batch systems. The variable volume flow systems we will consider later. Individual concentration can be determined by expressing volume as a function of conversion for a batch system. So this is one of the example of batch system we have said.

So you have impeller and you have some liquid and then you have another reactants, you have some reactant inside, so you have another reactant to feed in or both the mixtures of reactants can be feed at the beginning slowly and gradually you can start with the impeller and the reactions will proceed. So as you can see the volume will gradually change. The equations of state if it is a gas phase reaction then we can write

$$PV = ZN_TRT$$

So in this case the T is the temperature then P is the total pressure, Z is the compressibility factor and R is the universal gas constant, N_T is the total moles. So the relations which is given over here that is the equation of state is valid at any point in the system at any time. So this we can use at any time at any point in this system.

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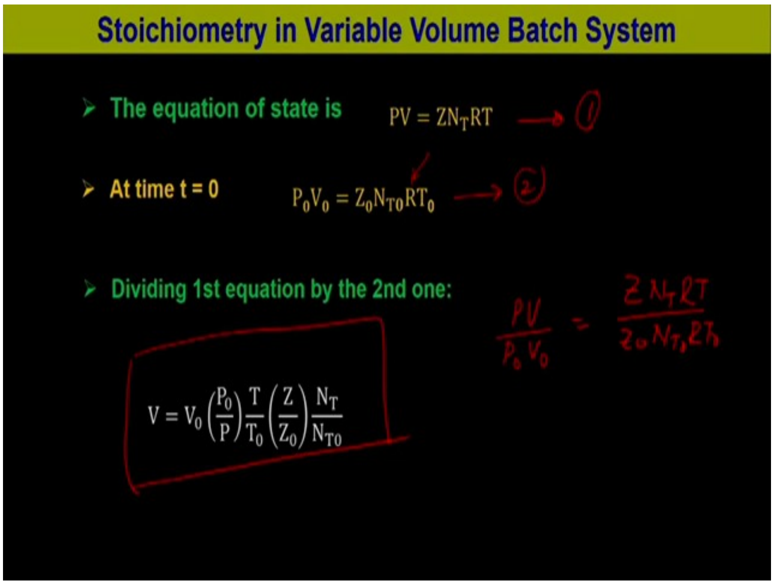

Stoichiometry in Variable Volume Batch System

- The equation of state is $PV = ZN_TRT \longrightarrow ①$
- At time t = 0 $P_0V_0 = Z_0N_{T0}RT_0 \longrightarrow ②$
- Dividing 1st equation by the 2nd one: $\frac{PV}{P_0V_0} = \frac{ZN_TRT}{Z_0N_{T_0}RT_0}$

$$\boxed{V = V_0\left(\frac{P_0}{P}\right)\frac{T}{T_0}\left(\frac{Z}{Z_0}\right)\frac{N_T}{N_{T0}}}$$

Now, equation of state is this

$$PV = ZN_TRT \text{ ....(1)}$$

At time t = 0, we can write

$$P_0V_0 = Z_0N_{T0}R_0T_0 \text{ ....(2)}$$

So as R is a universal gas constant it will not change, but all other parameters at t is equal to 0, P the total pressure should be P_0 that is the initial pressure, V would be at the beginning volume would be at V_0. Z the compressibility factor is Z_0 and total moles at the beginning is N_{T0} and temperature is T_0.

Now, if we divide this one, say this is equation (1) and this is equation (2), so if we divide (1) by (2), so we will obtain

$$\frac{PV}{P_0V_0} = \frac{ZN_TRT}{Z_0N_{T0}R_0T_0}$$

Now, if we rearrange this equation we will have

$$V = V_0(\frac{P_0}{P})(\frac{T}{T_0})(\frac{Z}{Z_0})(\frac{N_T}{N_{T0}})$$

So this is a relation between volume at two different conditions, two different time.

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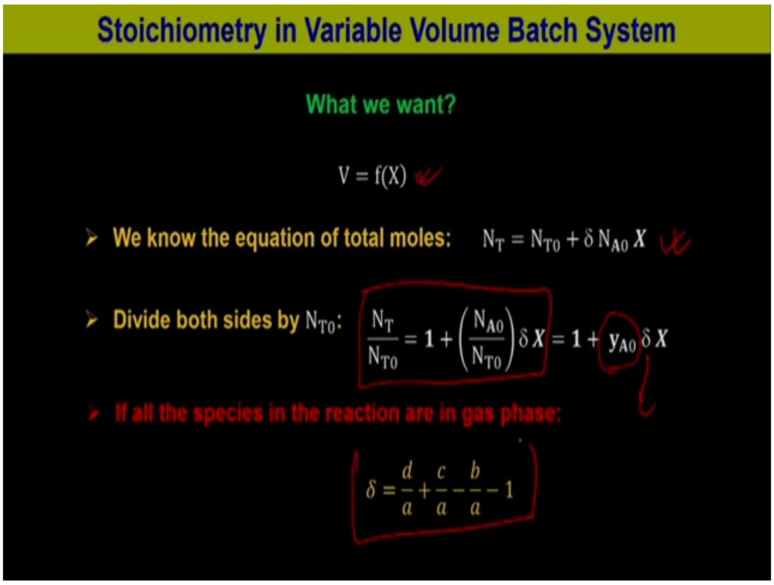

Stoichiometry in Variable Volume Batch System

What we want?

$V = f(X)$

- We know the equation of total moles: $N_T = N_{T0} + \delta N_{A0} X$
- Divide both sides by N_{T0}: $\frac{N_T}{N_{T0}} = 1 + \left(\frac{N_{A0}}{N_{T0}}\right)\delta X = 1 + y_{A0}\,\delta X$
- If all the species in the reaction are in gas phase:

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

Now, what we want? We want here volume as a function of conversion. So if we know volume as a function of conversion we can relate concentration in terms of volume and we replace the volume in terms of the conversion, so we can obtain the relations between concentration and conversion and then we can get the final relations between rate of reactions with conversion.

So we know the equation for total moles that is

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

So this is the equations of the total moles from the stoichiometric table. Now, if we divide both sides of this relations with N_{T0}, what will happen? This would be

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

so this relations we will obtain. So if we divide both sides with N_{T0}.

Then $\frac{N_{A0}}{N_{T0}}$ is nothing but y_{A0} as per the mole definition, so this would be the mole fractions.

So

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

So we have relations between N_{T0} and the conversion, $\frac{N_T}{N_{T0}}$ with conversion. Now, if all the species in the reactions are in the gas phase, this δ can be represented as we have seen before

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

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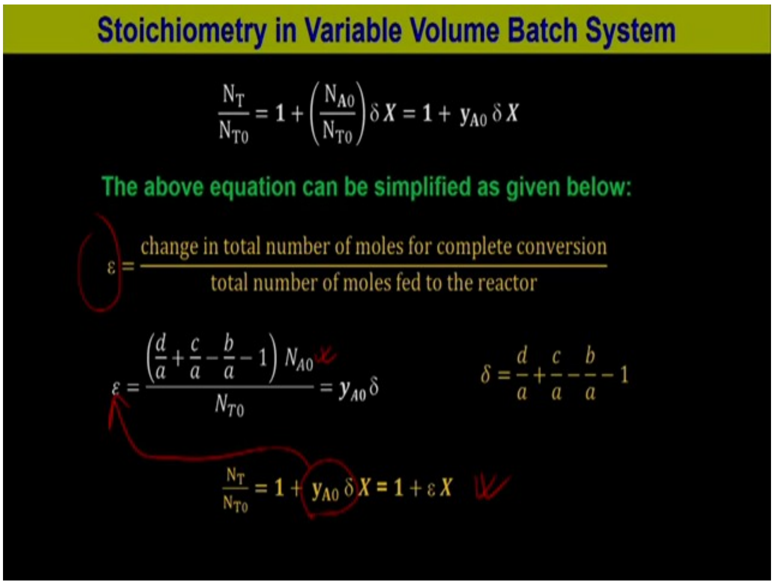

Stoichiometry in Variable Volume Batch System

$$\frac{N_T}{N_{T0}} = 1 + \left(\frac{N_{A0}}{N_{T0}}\right)\delta X = 1 + y_{A0}\,\delta X$$

The above equation can be simplified as given below:

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

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

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

So these relations we have and these equations can be simplified with definition of the ε which is nothing but

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

So this is a dimension less number, ε can be introduced and this equation can be simplified. So we can write

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

So the change in total moles for complete conversion would be, this is the change in total moles as

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

So this is delta and NA naught divided by NT naught. From the definition of ε you can write

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

So $y_{A0}\delta$ if we replace with ε this relations would be

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

And if we substitute this with ε so it would be

$$\frac{N_T}{N_{T0}} = 1 + \varepsilon X$$

So this is the relations between N_T and X.

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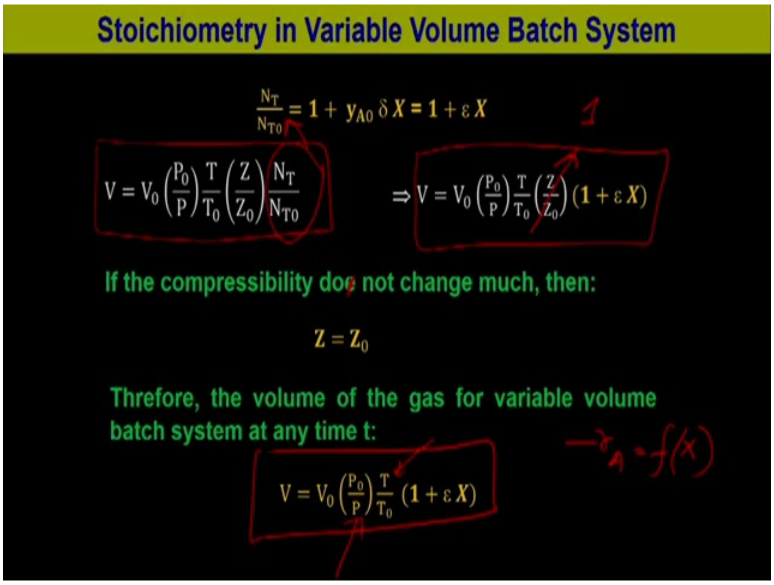

Stoichiometry in Variable Volume Batch System

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

1

$$V = V_0\left(\frac{P_0}{P}\right)\frac{T}{T_0}\left(\frac{Z}{Z_0}\right)\frac{N_T}{N_{T0}} \qquad \Rightarrow V = V_0\left(\frac{P_0}{P}\right)\frac{T}{T_0}\left(\frac{Z}{Z_0}\right)(1+\varepsilon X)$$

If the compressibility doe not change much, then:

$$Z = Z_0$$

Threfore, the volume of the gas for variable volume batch system at any time t:

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

$\rightarrow \gamma_A = f(X)$

Now we have derived these relations of the volume from the equations of state at two different time, at any time T and at time T is equal to zero about their state conditions and we know this relation,

$$V = V_0\left(\frac{P_0}{P}\right)\left(\frac{T}{T_0}\right)\left(\frac{Z}{Z_0}\right)\left(\frac{N_T}{N_{T0}}\right)$$

Now from here we can see that $\frac{N_T}{N_{T0}}$ this part if we replace with this then

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

So we have now the relation between volume and conversion.

Now, if the compressibility factor do not change much in that case we can write

$$Z = Z_0$$

so in that case we can write this volume at for the batch system at any time t can be written as

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

So this will be 1, so in that case we have the relations between volume with conversion at a particular temperature and pressure.

So once we fix the temperature and pressure we will have the relations between volume and conversion and then we can find out the relations between concentration and other conversion and then finally we will get $-r_A$ as a function of conversion. So this is how we can develop the Stoichiometry for variable volume batch systems. So thank you for your attention for hearing this lecture and we will continue our discussion of Stoichiometry for variable volume flow systems in the next lecture.