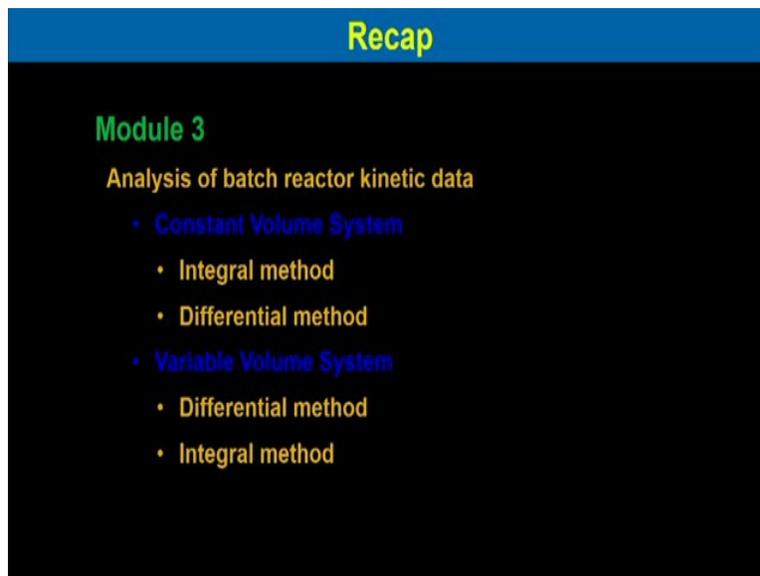


**Chemical Reaction Engineering-I**  
**Professor Bishnupada Mandal**  
**Department of Chemical Engineering**  
**Indian Institute of Technology Guwahati**  
**Lecture - 11**

**Introduction and Ideal Batch Reactor Design**

Welcome to the first lecture of module 4. In this module we will discuss the reactor design. Mostly we will consider ideal reactor design in this module. Before going to this lecture let us have brief recap on our previous lectures which we had in our module 3.

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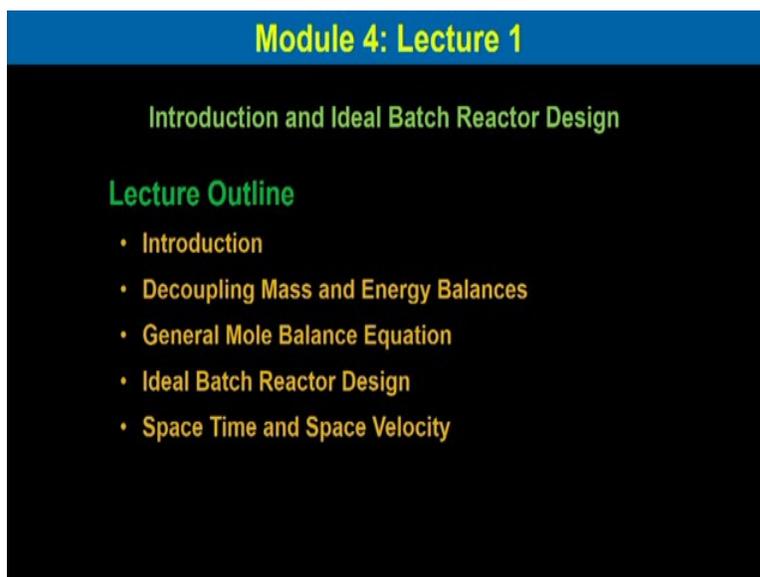


In module 3 basically we have considered analysis of the batch reactor Kinetic data. So several cases for the analysis of the batch reactor Kinetic data we have considered. First we have considered the constant volume system and we have considered two method of analysis, one is integral method of analysis and another one is differential method of analysis.

In integral method of analysis we have assumed a Kinetic rate loss and then we tested the integral form of the rate equations and we have seen whether that is fitted with the data obtained from the batch reactor data. In the differential form of analysis we have seen that we have taken the rate equations and we have directly fitted the data which we have obtained from the batch reactor.

And we have analyzed each methods merits and demerits like when the data is scattered we cannot use the differential method of analysis instead we can use the integral method of analysis. The other cases which we have considered is the variable volume systems and variable volume systems generally occur in case of the gas phase reactions in particular where the moles of the reactants and products varies before and after the reaction. And we have considered the differential method of analysis as well as the integral method of analysis.

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The slide features a blue header with the text "Module 4: Lecture 1" in yellow. Below the header, the text "Introduction and Ideal Batch Reactor Design" is displayed in green. Underneath, the heading "Lecture Outline" is also in green, followed by a bulleted list of five topics in yellow: "Introduction", "Decoupling Mass and Energy Balances", "General Mole Balance Equation", "Ideal Batch Reactor Design", and "Space Time and Space Velocity".

Now, in this lecture we will consider introduction to the reactor design and we will consider ideal batch reactor design in this lecture. The broad outline of this lecture would be introduction, then Decoupling mass and Energy balances, General mole balance equation and then we will consider Ideal batch reactor design, for batch reactor we will see the space time and space velocity, how they are related each other.

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**Introduction to Reactor Design**

**Basis:** Set of fundamental balance equations

**Equations:** Mathematical statement of physical laws

That requires

- Conservation of Mass
- Conservation of Momentum
- Conservation of Energy
- Conservation of quantities of particular chemical species

**What is the objectives?**

To know what size and type of reactor and method of operation are best for a given job.

So, introduction to the reactor design. The basis for designing any reactor is the set of fundamental balance equation. When we set of fundamental balance equations, what are these equations represents? These equations represents the mathematical statement of physical laws. So when we say mathematical statement of physical laws. What does it mean? The physical laws means it requires that the conservation of mass or conservation of momentum or conservation of energy.

In addition we can have conservation of quantities of particular chemical species which we wanted to follow for a particular reaction. What is the objectives then? Our prime objectives over here is to know what size and type of reactor and method of operations are the best for a given job. So we need to find out the reactor size and what type of reactor we need and the method of operation to obtain the best result for a given job. So with this basis we can start the ideal reactor design.

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**Introduction to Reactor Design**

**Albert E**

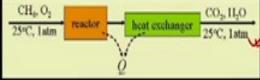
Einstein taught us that the mass and energy of a system are proportional; if a system loses energy its mass decreases; if it gains energy its mass increases.

**The relationship between mass and energy is:  $E = mc^2$**

Mass and energy are equivalent; they are simply different forms of the same entity.

Let's consider the combustion of methane, a highly exothermic chemical reaction:  $CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

Suppose 1 mole  $CH_4$  is completely burned with 2 mole  $O_2$  (16 g + 64 g = 80 g total):

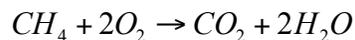


This reaction releases  $Q = 802$  kJ of energy, and so there is a corresponding decrease in mass of  $\sim 9$  ng ( $9 \times 10^{-8}$  g).

80.00000000 g reactants  $\longrightarrow$  79.99999991 g products

But before going to this let us have our great scientist Albert Einstein taught us that mass and energy of a system are proportional. That means if a system loses energy its mass decreases. If it gains energy its mass increases. So the relationship between the mass and energy is given is equal to  $E = mc^2$  which is well known equations. Now, from this relation we can see that mass and energy are equivalent and they are simply different forms of the same entity.

So let us consider the combustion of Methane. This reactions of combustion of Methane is a very high exothermic chemical reaction. As we can see Methane reacts with oxygen forms carbon dioxide and water.



So this reaction when occurs one mole of say if we consider one from the stoichiometry if we look into one mole of Methane is completely burned with two mole of Oxygen. If that is happened for complete combustion of Methane in presence of oxygen the stoichiometric amount of Oxygen will be used to burn one mole of Methane.

So it will take (16 + 64) gram so total 80 gram in total when it will react and it will form carbon dioxide and water-vapour. So the reaction scheme is given over here say Methane and oxygen at 25 degree centigrade and 1 atmosphere pressure it reacts in a reactor. Then this is exothermic

reactions so we need to take out the heat to keep the temperature same as it was before the reaction.

So to cool down to 25 degree centigrade and 1 atmosphere pressure so we are getting the product carbon dioxide and water at 25 degree centigrade and 1 atmosphere. So the amount of heat because of this highly exothermic reactions releases  $Q$  is equal to 802 kilo joule of energy.

So, if we consider this energy and if we apply this  $E = mc^2$  formula we can see that the corresponding decrease in the mass is about 9 nanogram, which is  $9 \times 10^{-9}$  gram. So, the mass change suppose if we start with 80 gram of total reactants it will give 79.999999991 gram product. So, the decrease of mass from 80 gram to  $9 \times 10^{-9}$  gram so 9 nanograms so which is very small.

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**Introduction to Reactor Design**

**Decoupling the Mass and Energy Balances**

Mass changes in chemical reactions (and all other chemical processes) are extremely small, usually much too small to even detect. We can therefore “decouple” mass and energy balances and make two separate assumptions:

- Mass is conserved in all chemical processes
- Energy is conserved in all chemical processes

For nuclear processes, this is not valid – the energy changes are huge and so the mass changes are significant.

Now, let us see that Decoupling of mass and energy balances. What does it mean? As we can see even if for very highly exothermic chemical reactions the mass changes in the chemical reactions are extremely small and usually much too small to even detect.

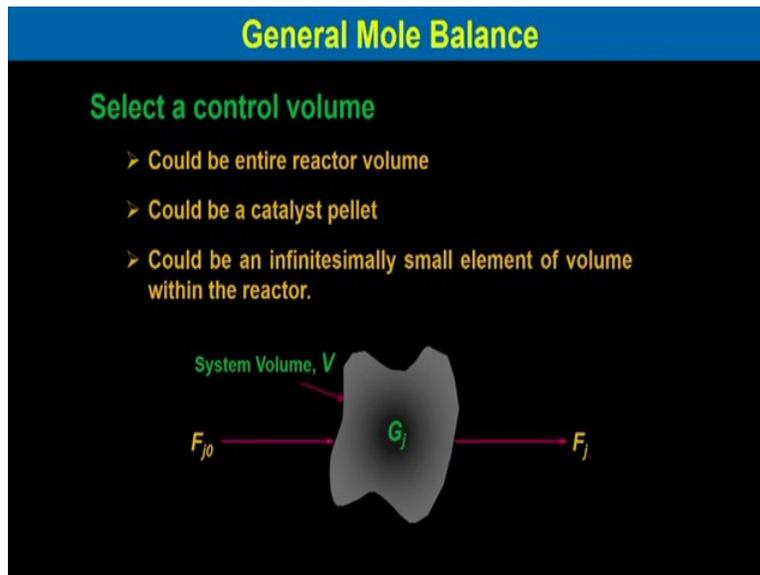
So, as we can see in the earlier examples of Methane combustion the mass change is  $10^{-9}$  gram,  $9 \times 10^{-9}$  gram which is 9 nanogram. It is very difficult to use any equipment to detect that small

change in the mass. So therefore, we can decouple the mass and energy balances and make two separate assumptions.

So we can make two separate assumptions. What are them? Mass is conserved in all chemical processes and energy is conserved in all chemical processes, with this assumptions that for highly exothermic chemical reactions in general the change of mass due to the chemical reactions is negligible or insignificant or it is difficult to detect.

So in that case we can assume this to separate assumptions. That is mass is conserved in all chemical processes and energy is conserved in all chemical processes. However, if we look into the nuclear reactions for nuclear processes this is not valid. This statement is not valid that means the energy changes are huge so that the mass changes are significant. So in that case for nuclear reactions we cannot decouple mass and energy balances.

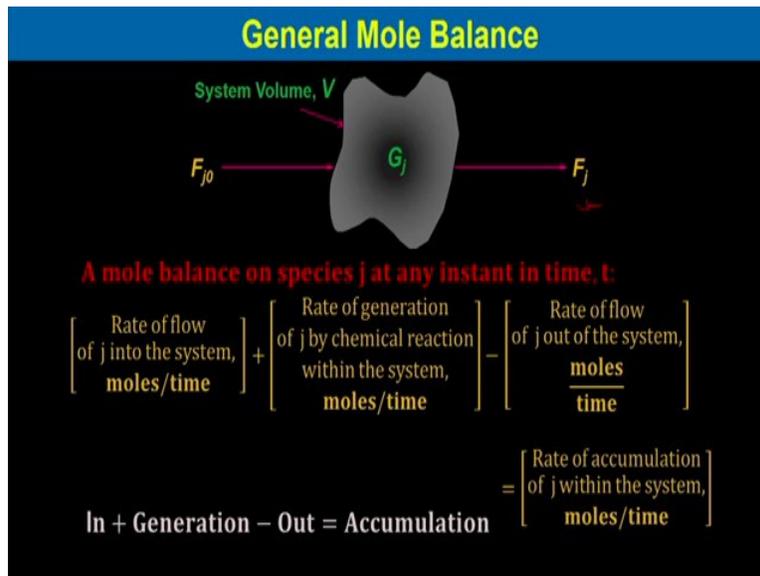
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Now, let us consider general mole balance, we need to select a control volume and that control volume could be an entire reactor volume. So we can take if it is gas phase reactions we consider entire reactor is the control volume or we can be consider as catalysts palette could be one reactor volume or control volume. Could be an infinitesimally small element of volume within the reactor.

So, we can consider very very small element inside the reactor as the control volume. So, let us consider this is our system volume or control volume whose volume is  $v$  and the feed entering the moles which is entering into this control volume in each  $F_{j0}$  and the mole which is going out is  $F_j$  and  $G_j$  is the amount which is generated due to the chemical reactions in this control volume.

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Now, let us do the mole balance. So if we do the mole balance for a species j at any instant in time T we can write

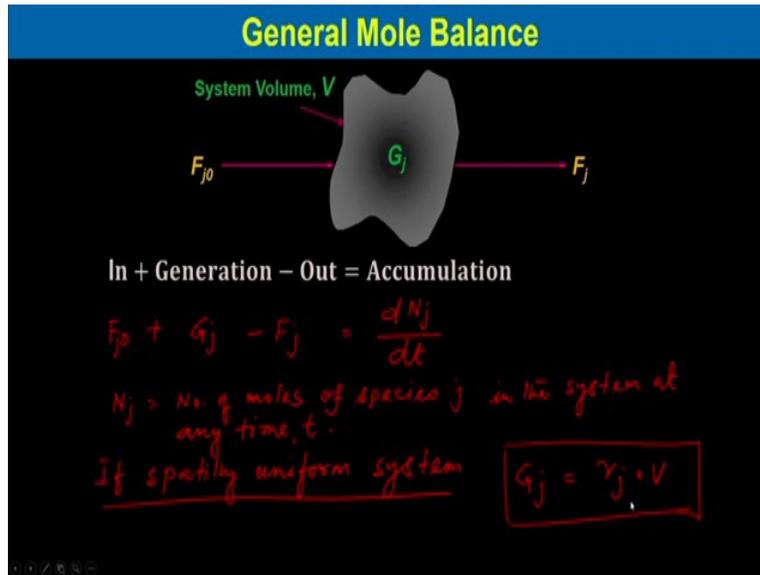
[rate of flow of j into the system i.e.  $F_{j0}$ ] + [rate of generation of any j component j by chemical reactions within the system] – [rate of flow out of j of the system] = [rate of accumulation of j within the system]

So rate of flow of J into the system which is in moles per time. This is also the generation  $G_j$  which is also in moles per time and the flow which is coming out from the reactor is also moles per time and the accumulation within the system should be moles per time as well so the unit should be same. So in simpler form this we can write

$$\text{In} + \text{Generation} - \text{Out} = \text{Accumulation}$$

So these are the simple mole balance equation for any species  $j$  at any instant  $T$ .

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Now, the overall mole balance equation is

$$\text{In} + \text{Generation} - \text{Out} = \text{Accumulation}$$

So in this case the In is  $F_{j0}$  plus Generation is  $G_j$  minus Out moles of the component out is  $F_j$  which is equal to the Accumulation. If  $N_j$  is the number of moles of species  $j$  in the system at any time anytime  $t$  then the accumulation term we can write  $\frac{dN_j}{dt}$ . Now, if this system is especially uniform that means so if it specially uniform system then we can write  $G_j$  would be equal to  $r_j$  rate of reactions of component  $j$  into the volume of the system. So for specially uniform system,

$$G_j = r_j \cdot V$$



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**General Mole Balance**

Consider  $M$  numbers of subvolumes

$$G_j = \sum_{i=1}^M \Delta G_{ji} = \sum_{i=1}^M r_{ji} \Delta V_i$$

Taking limit:  $M \rightarrow \infty$  and  $\Delta V \rightarrow 0$

$$G_j = \sum_{i=1}^M r_{ji} \Delta V_i = \int_V r_j dV$$

$i=1, \lim_{\Delta V \rightarrow 0, M \rightarrow \infty}$

$$F_{j0} + G_j - F_j = \frac{dN_j}{dt}$$

$$F_{j0} - F_j + \int_V r_j dV = \frac{dN_j}{dt}$$

General Mole balance eq<sup>n</sup>

Now, if we considered,  $M$  number of sub volumes say consider  $M$  numbers of sub volumes. So, if we  $M$  number of sub volumes we can write

$$G_j = \sum_{i=1}^M \Delta G_{ji} = \sum_{i=1}^M r_{ji} \Delta V_i$$

So, if you take the limit taking limit  $M$  tends to infinity and delta  $V$  tends to 0 very very small volume. If we take the these limits then we obtain

$$G_j = \sum_{i=1, \lim_{\Delta V \rightarrow 0, M \rightarrow \infty}}^M r_{ji} \Delta V_i$$

So integral

$$= \int_V r_j dV$$

So, then the balance equations which we have done earlier that is

$$F_{j0} + G_j - F_j = \frac{dN_j}{dt}$$

Now, if we substitute  $G_j$  over here we would obtain

$$F_{j0} - F_j + \int r_j dV = \frac{dN_j}{dt}$$

So this is the general mole balance equation. We will use this general mole balance equation for different ideal reactor design.

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**Ideal Batch Reactor**

$F_{j0} = F_j = 0$

$F_{j0} - F_j + \int_V r_j dV = \frac{dN_j}{dt}$

$\Rightarrow \frac{dN_j}{dt} = \int_V r_j dV$

Mole balance eqn for the batch reactor.

Let us consider ideal batch reactor design. So, if we consider ideal batch reactor which is fitted with a stirrer and this is filled. So initially this is charged with a feed and then it is closed. So this is not a flow system.

So in this case if  $F_{j0} = F_j = 0$ . So now, if we take the general mole balance equation that is

$$F_{j0} - F_j + \int_V r_j dV = \frac{dN_j}{dt}$$

So in this case if we apply this for the batch reactor then this would be 0, this is 0 so we would get from here

$$\frac{dN_j}{dt} = \int_V r_j dV$$

So this is the mole balance equation for the batch reactor.

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**Ideal Batch Reactor**

**For the reactant A**

$$N_A = N_{A0} - N_{A0} X_A = N_{A0} (1 - X_A)$$
$$\frac{dN_A}{dt} = -N_{A0} \frac{dX_A}{dt}$$

We know:

$$-r_A = -\frac{1}{V} \frac{dN_A}{dt} = \frac{N_{A0}}{V} \frac{dX_A}{dt}$$

Now, if you considered reactant A. For reactant A we can write the moles  $N_A$  would be equal to

$$N_A = N_{A0} - N_{A0} X_A$$

So while writing this we have considered a general reaction  $A \rightarrow B$ . So the conversion is  $X_A$ .

So this should be

$$= N_{A0}(1 - X_A)$$

So we can write  $dN_A$  from here. If we differentiate this would be equal to

$$\frac{dN_A}{dt} = -N_{A0} \frac{dX_A}{dt}$$

and we know

$$-r_A = -\frac{1}{V} \frac{dN_A}{dt}$$

Now if we substitute this  $\frac{dN_A}{dt}$  from here so you would obtain

$$-r_A = \frac{N_{A0}}{V} \frac{dX_A}{dt}$$

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**Ideal Batch Reactor**

$$-\frac{dN_j}{dt} = \int^V -r_j dV$$

For component A

$$N_{A0} \frac{dX_A}{dt} = \int_{\text{touch } \emptyset_1}^V -r_j dV$$

For perfectly mixed reaction mixture, there is no variation of  $(-r_j)$  with position.

$$\therefore \boxed{N_{A0} \frac{dX_A}{dt} = -r_j V}$$


So now, if we consider the general balance equation for the batch reactor that is

$$-\frac{dN_j}{dt} = -\int^V r_j dV$$

So if we substitute this one with for component A we can write

$$N_{A0} \frac{dX_A}{dt} = -\int^V r_j dV$$

Now, for a perfectly mixed reaction mixture, for perfectly mixed reaction mixture means this is homogeneously mixed, there is no variation of  $r_j$  with position, there is no variation of minus  $r_j$  with position. So then we can write from here therefore, we can write

$$N_{A0} \frac{dX_A}{dt} = -r_j V$$

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## Ideal Batch Reactor

### Rearrangement and Integration

$$N_{A0} \frac{dX_A}{dt} = -r_A V$$

$$\Rightarrow dt = N_{A0} \frac{dX_A}{(-r_A) V}$$

$$\Rightarrow \int_{t=0}^t dt = N_{A0} \int_{X_A=0}^{X_A} \frac{dX_A}{(-r_A) V} \Rightarrow t = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A) V}$$


\* General eq<sup>n</sup> showing time required to achieve a conversion  $X_A$  for Isothermal and Non-Isothermal.  
 \* The volume of reacting fluid and the rxn. rate remain under the integral sign.

Now, if we rearrange this equation and then if we integrate, so rearrangement and integration if we do we would obtain

$$N_{A0} \frac{dX_A}{dt} = -r_A V$$

$$\Rightarrow dt = N_{A0} \frac{dX_A}{-r_A V}$$

For component A it is  $r_A$ .

Now, if we integrate this so when  $t = 0$ ,  $X_A = 0$ . When  $t = t$ ,  $X_A$  is equal to  $X_A$ . So this is we will get,

$$\Rightarrow \int_{t=0}^t dt = N_{A0} \int_{X_A=0}^{X_A} \frac{dX_A}{-r_A V}$$

$$\Rightarrow t = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A) V}$$

So this is the general equation showing time required, time required to achieve a conversion  $X_A$ , to achieve conversion  $X_A$  for both cases isothermal and non-isothermal. And another feature for this we can see the volume of reacting fluid  $V$ . The volume of reacting fluid and the reaction rate remain under the integral sign. So this means that in general the rate of reactions and the volume

they change during the course of the reaction. Now, if we just plot these general equations for concentration versus or conversion versus time it will show a curve like this.

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**Ideal Batch Reactor**

**Limiting Cases**

$t = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)V}$

Case I: Constant density system  $\rightarrow V = \text{const.}$   
 $V = V_0$

$t = \frac{N_{A0}}{V} \int_0^{X_A} \frac{dX_A}{-r_A} = C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A} = - \int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$

$\epsilon_A = 0$

Case II: Density changes

$t = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)V_0(1+\epsilon_A X_A)} = C_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)(1+\epsilon_A X_A)}$

For any  $\epsilon_A$   $r_A = f(C)$

Now consider two limiting cases, in one case it is constant density system. If it is constant density system so our general equation says

$$t = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)V}$$

Case 1 constant density system. That means the volume is constant.

So this we can take out from here and we can write

$$t = \frac{N_{A0}}{V} \int_0^{X_A} \frac{dX_A}{-r_A}$$

or this would be equal to since  $V = V_0$  constant volume so this should be

$$= C_{A0} \int_0^{X_A} \frac{dX_A}{-r_A}$$

We can also write it is

$$= -\int_{C_{A0}}^{C_A} \frac{dC_A}{-r_A}$$

So for constant density system so your  $\varepsilon_A = 0$ .

Now, if density changes, Case 2 density changes. Then this

$$t = N_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)V_0(1 + \varepsilon_A X_A)}$$

So here we can write

$$= C_{A0} \int_0^{X_A} \frac{dX_A}{(-r_A)(1 + \varepsilon_A X_A)}$$

So this is applicable for both isothermal and non-isothermal systems and this is for any  $\varepsilon_A$  any change in volume, but in case of the non-isothermal system the variation of rate with temperature that is the function of temperature of  $r_A$  and the variation of temperature with the conversion that is  $X_A$  is function of temperature should be known to use this relation for non-isothermal system. So this is the two special cases for the batch reactor.

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**Space Time and Space Velocity**

Batch reactor: Reaction-time 't' is the natural performance measure of batch reactor.

space time  $\tau$ : Proper performance measure of the flow reactor.  
 space velocity:  $S$

**What space time?**

$$\tau = \frac{1}{S} = \left( \begin{array}{l} \text{time required to process one} \\ \text{reactor volume of feed measured} \\ \text{at specified condition} \end{array} \right) = [\text{time}]$$

**What space velocity?**

$$S = \frac{1}{\tau} = \left( \begin{array}{l} \text{Number of reactor volumes of feed} \\ \text{at specified conditions which can} \\ \text{be treated at unit time} \end{array} \right) = [\text{time}^{-1}]$$

So now, we will consider space time and space velocity, for the batch reactor we know the reaction time  $t$  is the natural performance measure of batch reactor. Space time and space velocity these two terms, these are the proper performance measure of the flow reactor.

Now, how to define space time? It is symbolized with  $\tau$  instead of  $t$  it is symbolizes with  $\tau$  and

the space velocity is represented with  $S$ . So which is  $\frac{1}{\tau}$  it is defined as time required to process 1 reactor volume of feed measured at specified condition. So this is unit of time as it is said the time required to process 1 reactor volume of feed measured at specified conditions. So condition has to be specified and the time required to process 1 reactor volume of it is the space time.

Now, for space velocity it can be defined as the similar way  $S$  would be equal to  $\frac{1}{\tau}$  which is the number of reactor volume that can be processed in unit time. So it is defined as number of reactor volume of feed at specified conditions, at specified conditions which can be treated at unit time. So the unit of this is  $\text{time}^{-1}$ . So as we can see this the reactor volumes of the feed should be mentioned at a particular conditions, that condition has to be specified so that we can define the space time and space velocity are based on a particular specified conditions.

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**Space Time and Space Velocity**

**What do you mean by space velocity  $5 \text{ hr}^{-1}$ ?**  
*This means that 5 reactor volumes of feed at specified conditions are being fed into or treated in the reactor per hour.*

**What do you mean by space time of 2 min?**  
*This means that every 2 min one reactor volume of the feed at specified conditions is being treated by the reactor.*

Now, what do you mean by space velocity of  $5 \text{ hrs}^{-1}$ ? This means that 5 reactor volumes of feed at specified conditions are being fed into or treated in the reactor per hour. So 5 reactor volumes of heat at specified conditions are being fed into the reactor or treated in the reactor per hour. So that indicates the space velocity of  $5 \text{ hrs}^{-1}$ .

Now, if we say what do you mean by space time of 2 minute? The space time of 2 minutes means, means that every 2 minute one reactor volume of the feed at specified conditions is being treated by the reactor. So this means at every 2 minutes one reactor volume of the feed at specified conditions is being treated by the reactor which is significance of space time of 2 minute.

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**Space Time and Space Velocity**

**On the basis of Entering Conditions**

We may arbitrarily select:

- temp.
- pressure
- state (gas, liq, solid)

If  $\tau$  and  $S$  are based on entering conditions to the reactor, then

$$\tau = \frac{1}{S} = \frac{C_{A0}V}{F_{A0}} = \frac{\frac{\text{Moles of A entering} \cdot \text{Volume of reactor}}{\text{Volume of feed}}}{\frac{\text{Moles of A entering}}{\text{time}}}$$

$$= \frac{\text{Volume of reactor}}{\text{Volume of feed/time}} = \frac{V}{v_0}$$

Now, we may arbitrarily select the temperature, pressure and state. So, for a particular feed we may arbitrarily select the temperature, the pressure and the state say gas, liquid or solid. So if the space time or space velocity they are on the basis of the entering conditions that means if  $\tau$  and  $S$  are based on entering conditions to the reactor then we can write

$$\tau = \frac{1}{S} = \frac{C_{A0}V}{F_{A0}}$$

That is

$$= \frac{\frac{\text{moles of A entering} \cdot \text{volume of reactor}}{\text{volume of feed}}}{\frac{\text{moles of A entering}}{\text{time}}}$$

So this should be

$$= \frac{\text{volume of reactor}}{\text{volume of feed / time}}$$

So this is  $\frac{V}{v_0}$ . So volume of the reactor divided by the volumetric flow rate.

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**Space Time and Space Velocity**

**On the basis of Standard Conditions**

*More convenient to measure the  $v_0$  at some standard state, specially when the reactor operates at numbers of temp.*

*Actual condition  $\rightarrow$  unprimed  
Standard condition  $\rightarrow$  primed.*

$$\tau' = \frac{1}{S'} = \frac{C'_{A0} V}{F_{A0}} = \tau \frac{C'_{A0}}{C_{A0}} = \frac{1}{S} \frac{C'_{A0}}{C_{A0}}$$

Now, it may be more convenient in certain cases to define the space time and space velocity at some standard conditions particularly when the reactor operates at various temperature. So more convenient to use to measure the volumetric flow rate that is  $v_0$  at some standard state. Especially when the reactor operates at numbers of temperature. For example, if we take some gaseous reactant which are fed to the reactor and which is at high temperature and then the same thing is liquid at the standard conditions so in that case, we should take care of the defining the state of the conditions.

Now, if we write the actual conditions which unprimed and standard conditions with primed, actual condition unprimed, standard condition primed. We can write

$$\tau' = \frac{1}{S'} = \frac{C'_{A0} V}{F_{A0}} = \tau \frac{C'_{A0}}{C_{A0}} = \frac{1}{S} \frac{C'_{A0}}{C_{A0}}$$

So this way we can relate between the actual conditions and the standard conditions space time and space velocity.

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So, thank you very much for attending this lecture and we will continue the reactor design for other idealized reactor in the next lecture.