Polymer Reaction Engineering
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Lecture-18
Design Equation for ideal Reactors

Welcome to the concept of design equation for ideal reactors. Before we go into deep let us have looked at what we studied in the previous lectures. We performed so many calculations and so many derivations for the interpretation of batch reactor data.

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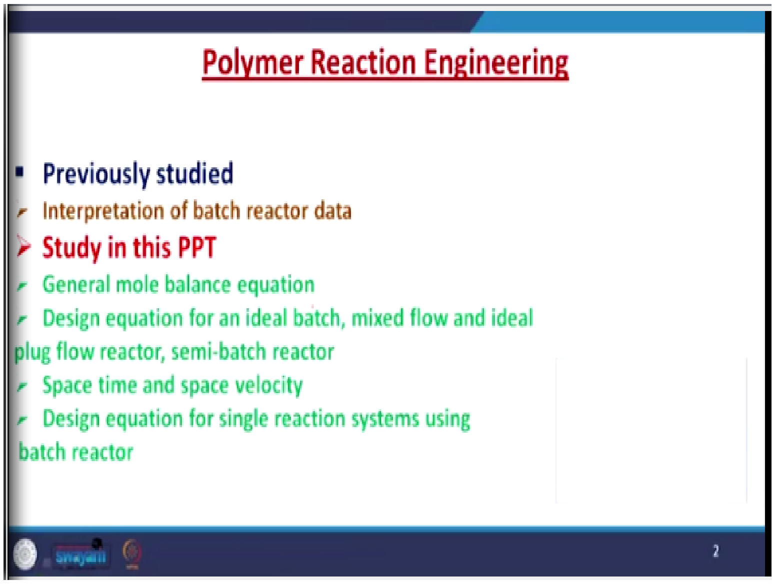

Polymer Reaction Engineering

- Previously studied
- Interpretation of batch reactor data
- Study in this PPT
- General mole balance equation
- Design equation for an ideal batch, mixed flow and ideal plug flow reactor, semi-batch reactor
- Space time and space velocity
- Design equation for single reaction systems using batch reactor

And as well as those who are the equations are required for designing the polymer reaction reactors plus polymerization processes. And all these things are in-situ with the various kind of a polymerization schemes maybe the solution polymerization maybe the emulsion polymerization etc. Now in this particular lecture we are going to study about the concept of general mole balance equation.

All these equations are of course the mathematical equations, we will discuss about the design equation for any ideal batch reactor, mixed flow reactor, ideal PFR, semi batch reactor etc. We will have a basic concept of space time and space velocity you know that both the things are extremely important for handling the reactors, various kind of reactors those who are in question with the polymer reaction engineering.

We will develop several design equations for single reactant system using batch reactors. So, let us have start with the general mole balance equation, now you see that here we have just given a blog diagram about the general for the prediction of mole balance equation. So, for mole balance of any species ‘i’ on the system volume where ‘i’ represent a particular chemical species, suppose n number of species are taking part in a particular reactor.

And there may be different species like A, B, C, D etc. Now here you can represent any individual species like i maybe j, k etc. Now this is if you talk in terms of reaction engineering or if you talk in terms of thermodynamics, this is the microscopic level apart from the macroscopic concept.

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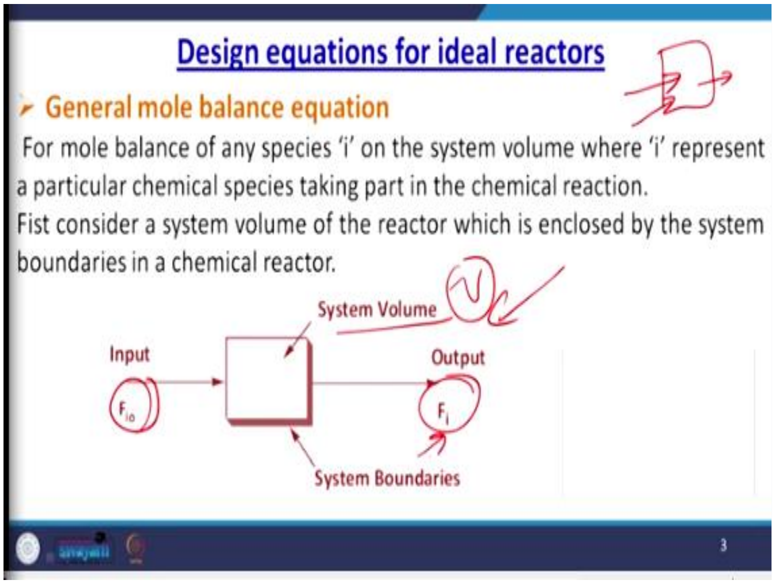

Design equations for ideal reactors

- General mole balance equation

For mole balance of any species ‘i’ on the system volume where ‘i’ represent a particular chemical species taking part in the chemical reaction.

Fist consider a system volume of the reactor which is enclosed by the system boundaries in a chemical reactor.

So, let us have that this mole balance we are in the interest of any species i in terms of developing the mole balance equation. So, anything which is participating in this particular reaction mass there are 2 streams, one is that input stream, another one is output stream. So, if we consider a system volume related to the reactor which is usually enclosed by boundaries in chemical reaction.

Now as you know then thermodynamically the boundaries are three different types isolated, open and permeable. Now here then if you see that this particular reaction where the system volume is having say V and you are having the stream that is F_{io}. That is the start of your i^{th} species and after say time interval t and crossing the system volume V it is having the flow rate of i, F_i.

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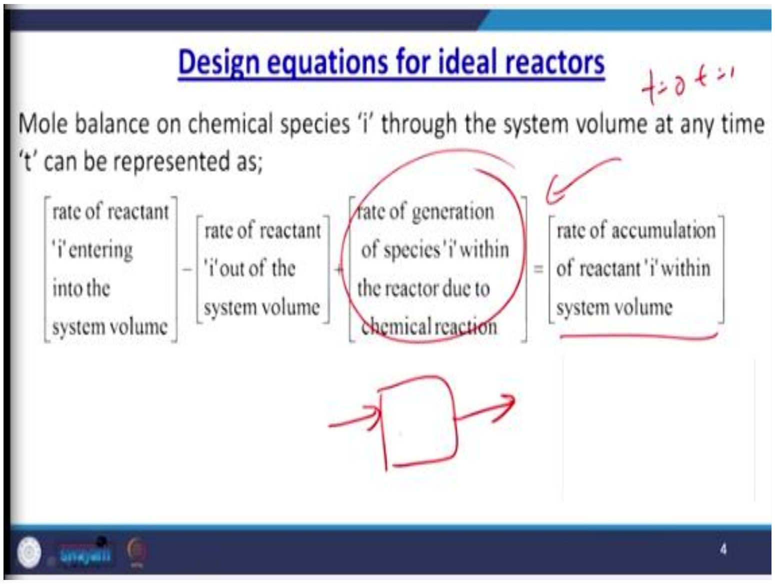

Design equations for ideal reactors

t=0 t=1

Mole balance on chemical species 'i' through the system volume at any time 't' can be represented as;

$$\begin{bmatrix}\text{rate of reactant}\\ \text{'i' entering}\\ \text{into the}\\ \text{system volume}\end{bmatrix} - \begin{bmatrix}\text{rate of reactant}\\ \text{'i' out of the}\\ \text{system volume}\end{bmatrix} + \begin{bmatrix}\text{rate of generation}\\ \text{of species 'i' within}\\ \text{the reactor due to}\\ \text{chemical reaction}\end{bmatrix} = \begin{bmatrix}\text{rate of accumulation}\\ \text{of reactant 'i' within}\\ \text{system volume}\end{bmatrix}$$

Now the mole balance equation you can develop with respect to the chemical species through the system volume and if you are having time t, from t = 0 to t = 1. So, the rate of reactant i usually into entering into the system volume minus the rate of reactant i out of the system volume. This is then the rate of a generation of species i within the reactor due to the chemical reaction is equal to the rate of accumulation of reactant i within the system volume.

$$\begin{bmatrix}\text{rate of reactant}\\ \text{'i' entering}\\ \text{into the}\\ \text{system volume}\end{bmatrix} - \begin{bmatrix}\text{rate of reactant}\\ \text{'i'out of the}\\ \text{system volume}\end{bmatrix} + \begin{bmatrix}\text{rate of generation}\\ \text{of species 'i'within}\\ \text{the reactor due to}\\ \text{chemical reaction}\end{bmatrix} = \begin{bmatrix}\text{rate of accumulation}\\ \text{of reactant 'i'within}\\ \text{system volume}\end{bmatrix}$$

Now you see in this particular mathematical equation we have encountered all kind of approaches that is how much i th species being consumed in due course of time during the reaction, how much rate is there of reactant i into the system volume which is entering and which is going out**.** So, we have considered all approaches of species i in their particular reaction stream.

$$\Rightarrow \qquad F_{i_o} - F_i + G_{io} = \frac{dN_i}{dt}$$

Now if we try to put this entire scheme mathematically then we can write the mole balance of chemical species like this that F_{i0} - F_i which is this one + G_{i0} that is the rate of a generation of species i within the reactor due to the chemical reaction and it is dN_i upon dt, so the rate of generation of space is i usually given by $G_i = r_iV$.

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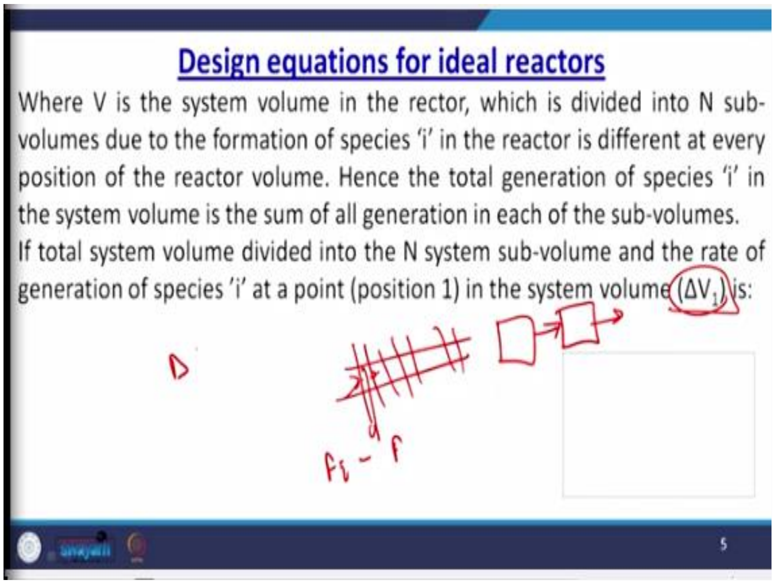

Design equations for ideal reactors

Where V is the system volume in the rector, which is divided into N sub-volumes due to the formation of species 'i' in the reactor is different at every position of the reactor volume. Hence the total generation of species 'i' in the system volume is the sum of all generation in each of the sub-volumes.

If total system volume divided into the N system sub-volume and the rate of generation of species 'i' at a point (position 1) in the system volume (ΔV_1) is:

Now if we consider that V is the system volume in the reactor which is usually divided into N sub volume due to the formation of various species in i in the reactor. And sometimes it is different at every position of the reactor volume; sometimes you may need to have a sequential approach like one output is the input of another one. And sometimes these things are integrated within the specified volume.

So, if we talk about the total generation of species i in the system volume, it is usually sum of all generations in each of sub volumes. So, if we consider that a total volume which needs to be divided into n different type of sub volume and the rate of a generation of species i at any point of time or any position 1; that is sometimes referred as delta V_1.

$$G_{i1} = r_{i1} \Delta V_1$$

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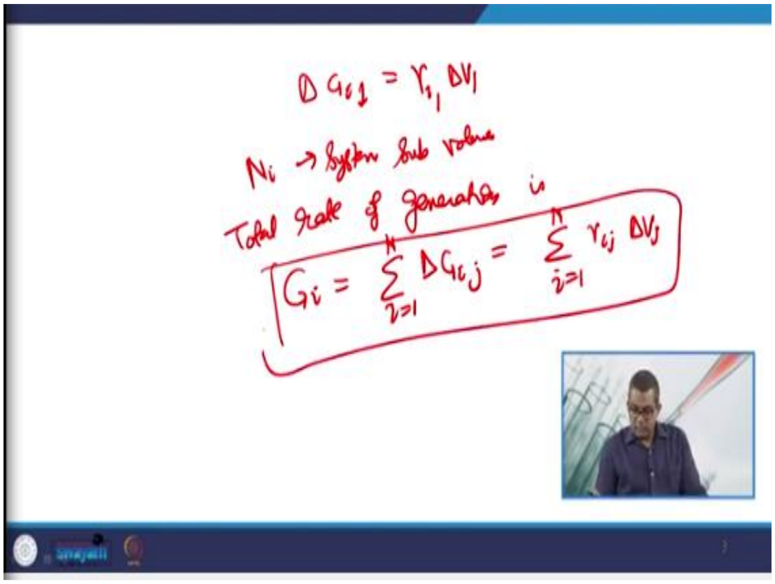

$\Delta G_{i1} = r_{i1} \Delta V_1$

$N_i \rightarrow$ System sub volume

Total rate of generation is

$$\boxed{G_i = \sum_{j=1}^{N} \Delta G_{ij} = \sum_{j=1}^{N} r_{ij} \Delta V_j}$$

So, this can be represented as delta G_i 1. Now if there are N_i systems these are the system sub volumes, then the total rate of generation is summation i. Now this is the total rate of generation for this particular system.

The total rate of generation

$$G_i = \sum_{j=1}^{M} \Delta G_{ij} = \sum_{j=1}^{M} r_{ij}\, \Delta V_j$$

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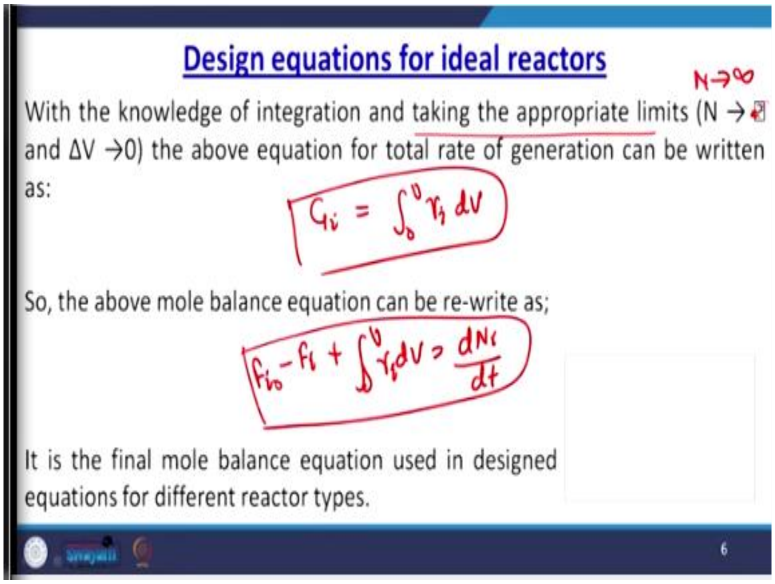

Design equations for ideal reactors

$N \rightarrow \infty$

With the knowledge of integration and taking the appropriate limits (N → ∞ and ΔV → 0) the above equation for total rate of generation can be written as:

$$\boxed{G_i = \int_0^V r_i \, dV}$$

So, the above mole balance equation can be re-write as;

$$\boxed{F_{i0} - F_i + \int_0^V r_i \, dV = \frac{dN_i}{dt}}$$

It is the final mole balance equation used in designed equations for different reactor types.

Now with the knowledge of integration and sometimes I need to take the appropriate limit like N tends to infinity and delta V tends to 0. This equation which we discussed previously regarding the total rate of generation it can be written as mu. So, this mole balance equation again if we wish to rearrange the things and if you wish to rewrite that particular equation it can be rewritten as with respect to the over here.

Total rate of generation is therefore

$$\Rightarrow \quad G_i = \int_0^V r_i dV$$

So the above mole balance equation can be re-write as;

$$\Rightarrow \quad F_{i_o} - F_i + \int_0^V r_i dV = \frac{dN_i}{dt}$$

It is the final mole balance equation used in designed equations for different reactor types.

Now this is the final mole balance equation and the designed equation for different reactor types. Now let us have a consideration to different type of ideal reactors, now here the ideal batch reactor the concept of ideal batch reactor that we have to design the performance equation for homogeneous reacting system or for single fluid reacting in the ideal reactor which is further being used for isothermal or non isothermal equation. If you recall that in the previous lecture we discussed about the equimolar and non equimolar type of system.

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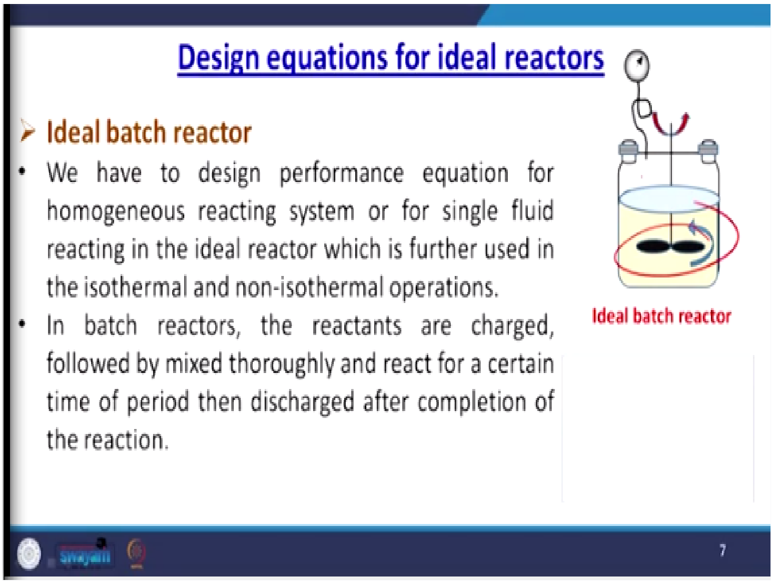

Design equations for ideal reactors

Ideal batch reactor

- We have to design performance equation for homogeneous reacting system or for single fluid reacting in the ideal reactor which is further used in the isothermal and non-isothermal operations.
- In batch reactors, the reactants are charged, followed by mixed thoroughly and react for a certain time of period then discharged after completion of the reaction.

Ideal batch reactor

Now in batch reactor the reactants are usually charged followed by if you see here followed by mix thoroughly or rigorously depending upon the scenario. And react for a certain period of time and then discharge after completion of the reaction; this is the basic definition of your batch reactor. Now as the composition of a product changes with the time in the reactor there is an unsteady type of operation and referred as unsteady state operation.

So, the composition throughout the reactor is remaining constant at any particular point of time. There are various applications associated with this type of reactor system, it is used for the testing of a new process which is not yet fully developed because see our benchmarking is this one.

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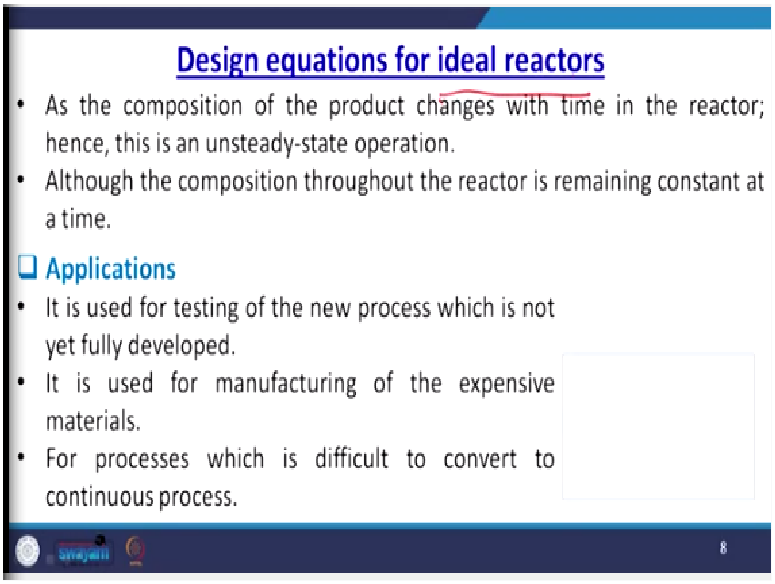

Design equations for ideal reactors

- As the composition of the product changes with time in the reactor; hence, this is an unsteady-state operation.
- Although the composition throughout the reactor is remaining constant at a time.

❑ Applications

- It is used for testing of the new process which is not yet fully developed.
- It is used for manufacturing of the expensive materials.
- For processes which is difficult to convert to continuous process.

It is used for the manufacturing of all kind of expensive materials, sometimes because of the limitation in the continuous type of a reactor, this is more feasible. For processes which is difficult to convert into continuous processes. There are various advantages and disadvantages associated with this type of reactor system, it has advantageous that being high conversion of a reactant after leaving the material in the reactor for a longer period of time. But there are certain disadvantages associated with this reactor that it requires higher labor cost for charging, discharging and cleaning per batch.

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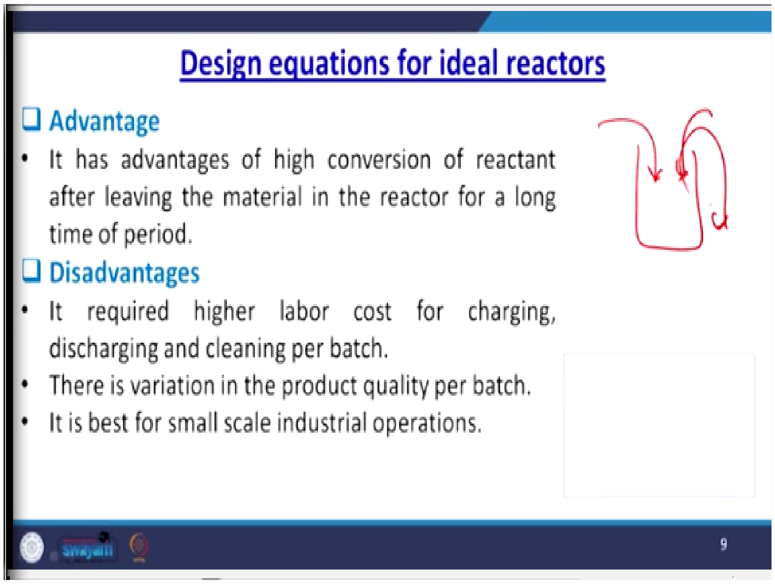

Design equations for ideal reactors

❑ Advantage

- It has advantages of high conversion of reactant after leaving the material in the reactor for a long time of period.

❑ Disadvantages

- It required higher labor cost for charging, discharging and cleaning per batch.
- There is variation in the product quality per batch.
- It is best for small scale industrial operations.

Because you need to put the entire mass over here and then you need to discharge the things, so thereby it creates a lot of economic burden to the system. There is a variation in the product quality per batch and sometimes there may be a chance of formation of stagnant zones within the reactor mass, that is why it is best suited for small scale industrial operation. Now let us have a look about the design equation for batch reactors, usually the inflow and outflow of the reactants or a product they are not allowed during the process of a reaction.

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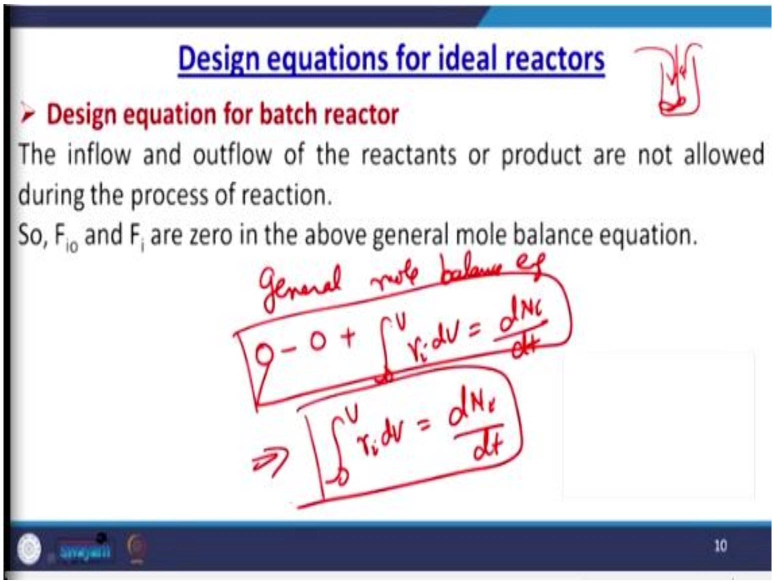

Design equations for ideal reactors

- **Design equation for batch reactor**

The inflow and outflow of the reactants or product are not allowed during the process of reaction.

So, F_{i0} and F_i are zero in the above general mole balance equation.

General mole balance eq

$$\boxed{0 - 0 + \int_0^V r_i dV = \frac{dN_i}{dt}}$$

$$\Rightarrow \boxed{\int_0^V r_i dV = \frac{dN_i}{dt}}$$

As you refer to this particular batch reactor, so if we say that F_{i0} and F_i they are 0 the generalized mole balance equation which we developed in earlier concept. So, the general mole balance equation, we can write as which is dN_i upon dt or so this is the general mole balance equation. Now the reacting material is perfectly mixed throughout the reactor, so there is no change in the rate of a reaction in the reactor and volume. Therefore, the required performance equation in the batch reactor is usually given by.

$$\Rightarrow \quad 0 - 0 + \int_0^V r_i \mathrm{dV} = \frac{\mathrm{dN}_i}{\mathrm{dt}}$$

So, the required performance equation for the batch reactor is

$$\Rightarrow \quad \mathrm{r}_i V = \frac{\mathrm{dN}_i}{\mathrm{dt}}$$

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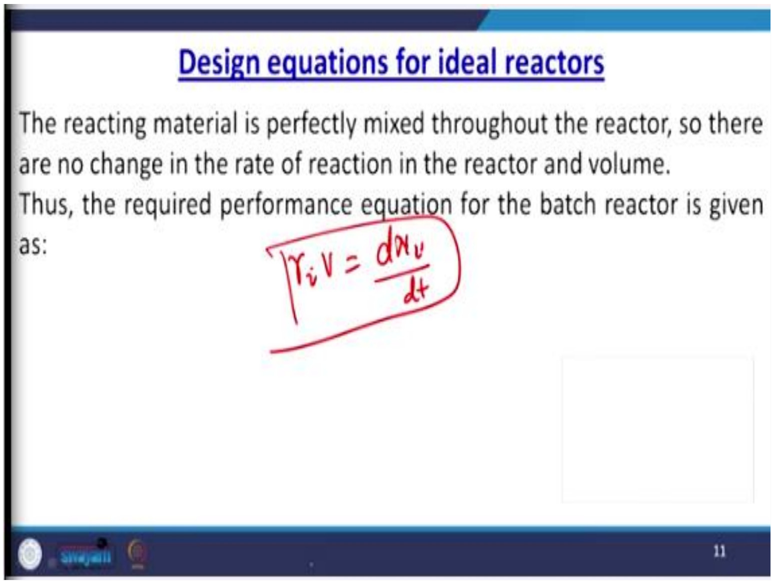

Design equations for ideal reactors

The reacting material is perfectly mixed throughout the reactor, so there are no change in the rate of reaction in the reactor and volume.

Thus, the required performance equation for the batch reactor is given as:

$$\boxed{r_i V = \frac{dx_v}{dt}}$$

So, this is our required performance equation which is quite useful for the system. Now let us have a look about the various design equations for ideal reactors. So, the design equation for any ideal mixed flow reactor or CSTR continuous tank reactors sometimes referred as this one.

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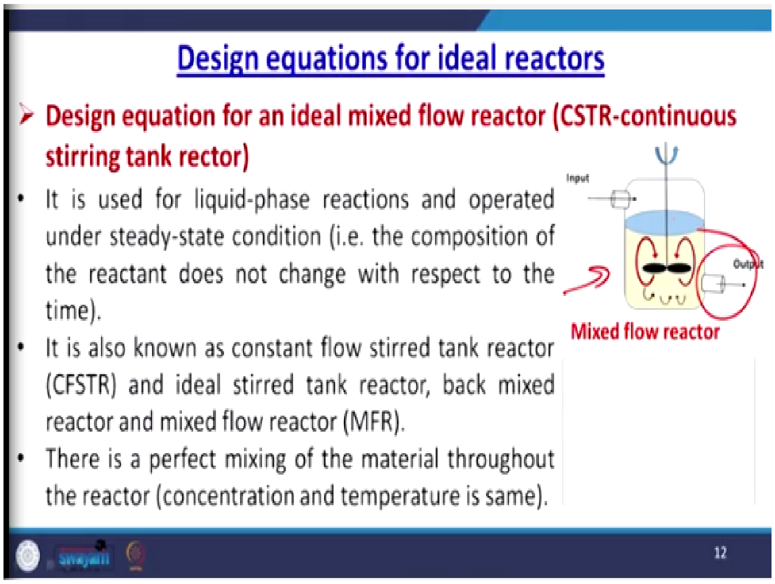

Design equations for ideal reactors

- **Design equation for an ideal mixed flow reactor (CSTR-continuous stirring tank rector)**
  - It is used for liquid-phase reactions and operated under steady-state condition (i.e. the composition of the reactant does not change with respect to the time).
  - It is also known as constant flow stirred tank reactor (CFSTR) and ideal stirred tank reactor, back mixed reactor and mixed flow reactor (MFR).
  - There is a perfect mixing of the material throughout the reactor (concentration and temperature is same).

Mixed flow reactor

So, it is used for the liquid phase reaction and operated under steady state condition. And this condition prevails that the composition of the reactant does not change with respect to the time. And it is also known as a continuous fluid flow listed tank reactor and ideal street tank reactor back mix reactor and a mixed flow reactor. So, these are the common names in the reaction engineering. Now there is a perfect mixing of a material throughout the reactor therefore the concentration and the temperature they are supposed to be constant throughout. So, if we take the temperature and concentration in the reactor same as in the exit stream, this is my exit stream.

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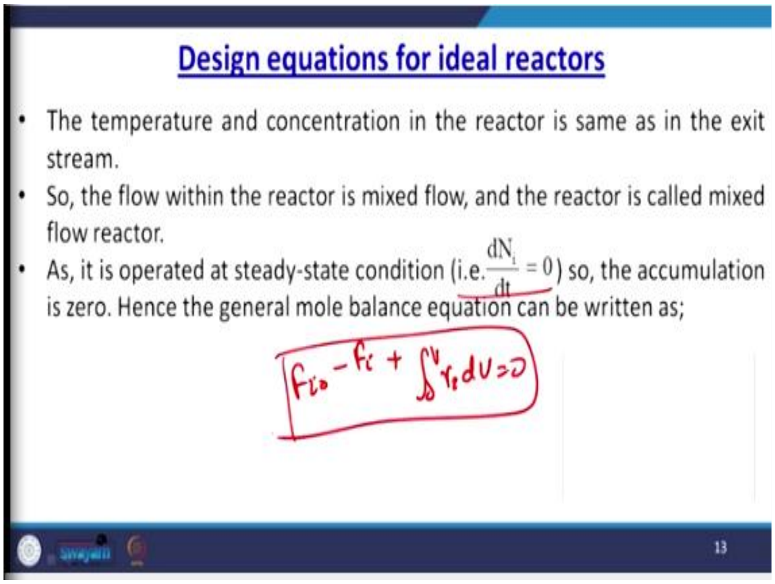

Design equations for ideal reactors

- The temperature and concentration in the reactor is same as in the exit stream.
- So, the flow within the reactor is mixed flow, and the reactor is called mixed flow reactor.
- As, it is operated at steady-state condition (i.e. $\frac{dN_i}{dt} = 0$) so, the accumulation is zero. Hence the general mole balance equation can be written as;

$$\boxed{F_{io} - F_i + \int_0^V r_i \, dV = 0}$$

Therefore, the flow within the reactor is mixed flow, and the reactor is called the mix flow reactor. It is operated under the steady state condition, that is dN_i upon dt = 0, so accumulation is 0. And the general mole balance equation can be written as F_i because the accumulation term is in this case is 0.

Hence the general mole balance equation can be written as;

$$\Rightarrow \qquad F_{i_o} - F_i + \int_0^V r_i \, dV = 0$$

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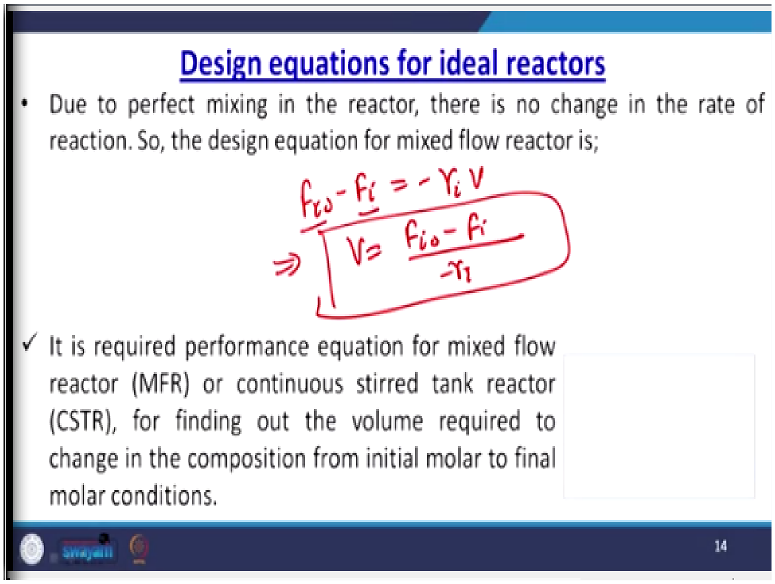

Design equations for ideal reactors

- Due to perfect mixing in the reactor, there is no change in the rate of reaction. So, the design equation for mixed flow reactor is;

$$F_{i0} - F_i = -r_i V$$

$$\Rightarrow \boxed{V = \frac{F_{i0} - F_i}{-r_i}}$$

✓ It is required performance equation for mixed flow reactor (MFR) or continuous stirred tank reactor (CSTR), for finding out the volume required to change in the composition from initial molar to final molar conditions.

Now due to perfect mixing in the reactor there is no change in the rate of a reaction. Therefore, the design equation for MFR or mixed flow reactor can be written as or F_i upon. Now this is the required performance equation for MFR or CSTR for finding out the volume required to change in the composition from initial molar to the final molar conditions.

$$F_{i_o} - F_i = r_i V$$

$$\Rightarrow \qquad V = \frac{F_{i_o} - F_i}{r_i}$$

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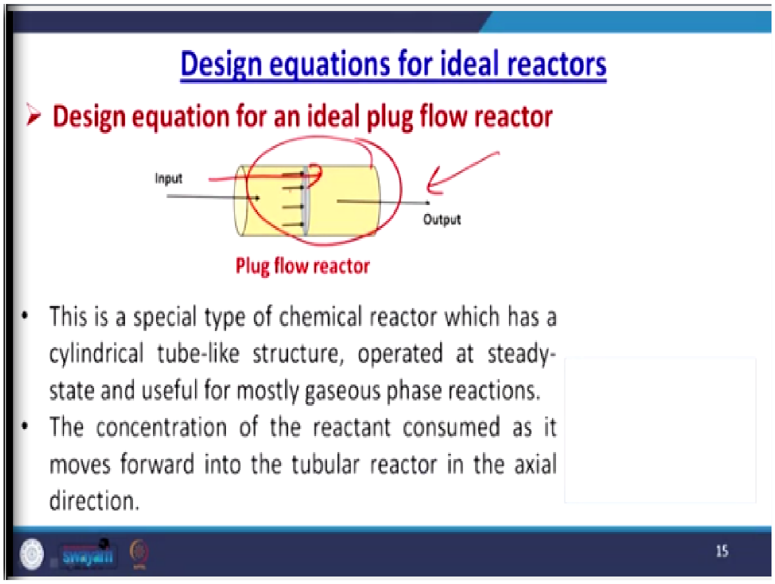

Design equations for ideal reactors

➢ Design equation for an ideal plug flow reactor

Plug flow reactor

- This is a special type of chemical reactor which has a cylindrical tube-like structure, operated at steady-state and useful for mostly gaseous phase reactions.
- The concentration of the reactant consumed as it moves forward into the tubular reactor in the axial direction.

Now let us have a look about the PFR, the plug flow reactor. Now this is the simplest diagram of the plug flow reactor. This is a special type of a chemical reactor which has a cylindrical tube-like structure operated at a steady state. And it is very useful for various gaseous phase reaction when you require the gaseous phase reaction need to be performed, then it is a very useful reaction for this. Now the concentration of the reactant consumed as it moves forward into the tubular reactor in the axial direction.

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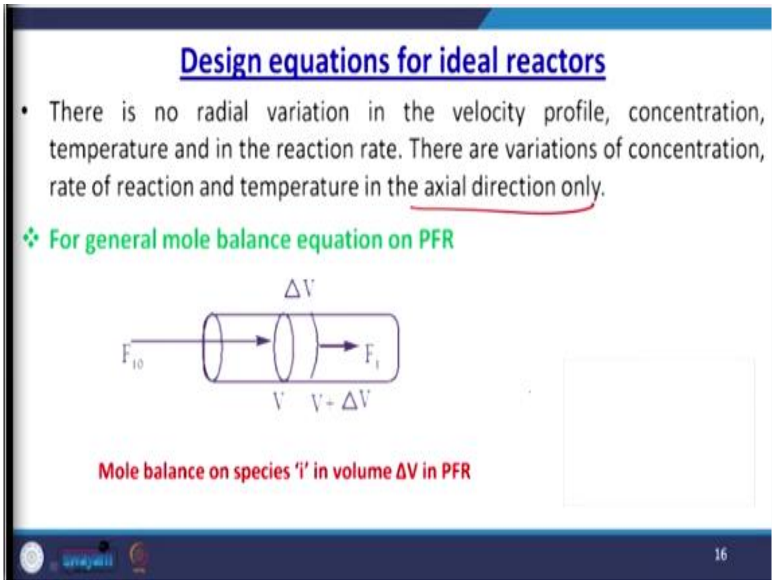

Design equations for ideal reactors

- There is no radial variation in the velocity profile, concentration, temperature and in the reaction rate. There are variations of concentration, rate of reaction and temperature in the axial direction only.

❖ For general mole balance equation on PFR

Mole balance on species 'i' in volume ΔV in PFR

Now there is no radial variation in the velocity profile, concentration, temperature in the reaction rate. Now there are variation in concentration rate of reaction and a temperature in axial direction only. If you see that this is the typical anatomy of general mole balance equation of a PFR.

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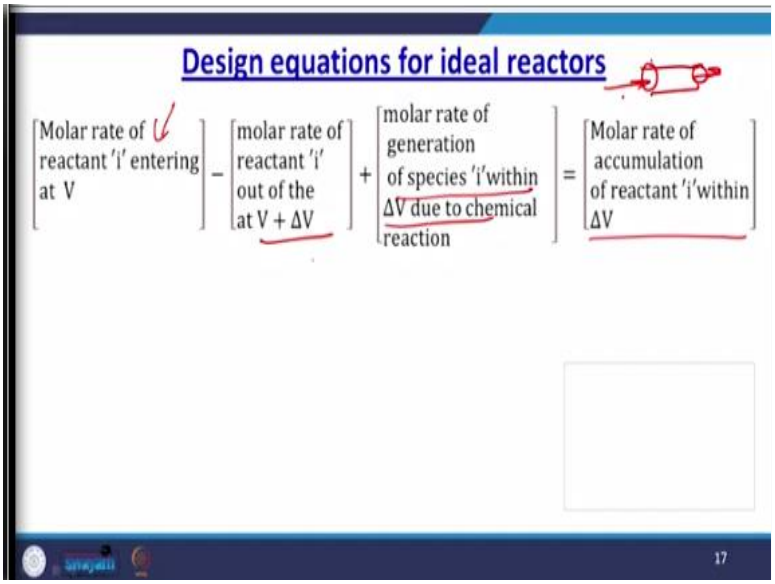

Design equations for ideal reactors

$$\begin{bmatrix}\text{Molar rate of}\\ \text{reactant 'i' entering}\\ \text{at V}\end{bmatrix} - \begin{bmatrix}\text{molar rate of}\\ \text{reactant 'i'}\\ \text{out of the}\\ \text{at V} + \Delta\text{V}\end{bmatrix} + \begin{bmatrix}\text{molar rate of}\\ \text{generation}\\ \text{of species 'i'within}\\ \Delta\text{V due to chemical}\\ \text{reaction}\end{bmatrix} = \begin{bmatrix}\text{Molar rate of}\\ \text{accumulation}\\ \text{of reactant 'i'within}\\ \Delta\text{V}\end{bmatrix}$$

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Now here if we wish to write the design equation then the starting point is that mole rate of any reactant i at the entrance just, I am drawing this PFR again at entering.

$$\begin{bmatrix}\text{Molar rate of}\\ \text{reactant 'i' entering}\\ \text{at V}\end{bmatrix} - \begin{bmatrix}\text{molar rate of}\\ \text{reactant 'i'}\\ \text{out of the}\\ \text{at V} + \Delta\text{V}\end{bmatrix} + \begin{bmatrix}\text{molar rate of}\\ \text{generation}\\ \text{of species 'i'within}\\ \Delta\text{V due to chemical}\\ \text{reaction}\end{bmatrix} = \begin{bmatrix}\text{Molar rate of}\\ \text{accumulation}\\ \text{of reactant 'i'within}\\ \Delta\text{V}\end{bmatrix}$$

Then the mole rate of reactant i at the outlet that sometimes it may be represented as V + delta V + molar rate of generation of species i within this delta V due to the any kind of a chemical reaction. And last is the molar rate of accumulation of reactant i within that particular change in volume. So, the general mole balance equation we can write like this.

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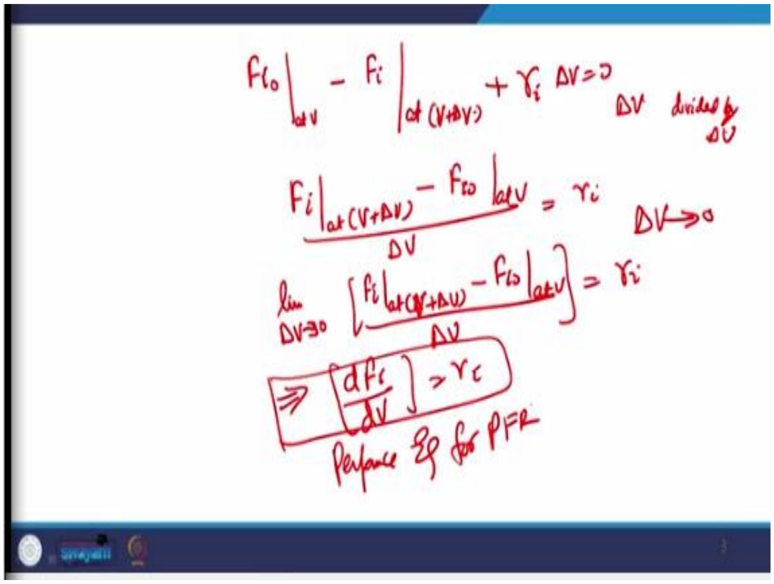

$$F_{i_0}\Big|_{at\,V} - F_i\Big|_{at\,(V+\Delta V)} + r_i\,\Delta V = 0$$

ΔV divided by ΔV

$$\frac{F_i\big|_{at\,(V+\Delta V)} - F_{i_0}\big|_{at\,V}}{\Delta V} = r_i \qquad \Delta V \to 0$$

$$\lim_{\Delta V \to 0}\left[\frac{F_i\big|_{at\,(V+\Delta V)} - F_{i_0}\big|_{at\,V}}{\Delta V}\right] = r_i$$

$$\boxed{\Rightarrow \left[\frac{dF_i}{dV}\right] = r_i}$$

Perfomance Eq for PFR

At V - F_i at V + delta V, now if we divide both the sides with the delta V and rearrange the things, then we have upon delta V. Now if we take the things like delta V tends to 0 then tends to 0 delta V or this refers to d F_i upon dV. Now this is the required differential form of performance equation for any PFR. Now let us have a due consideration to the space time and space velocity.

$$\Rightarrow \qquad F_{i_o}\text{at (V)} - F_i \text{ at } (V + \Delta V) + r_i \Delta V = 0$$

On dividing by ΔV on both side of the above equation, rearranging then we have

$$\Rightarrow \qquad \left[\frac{F_{i \text{ at } (V+\Delta V)} - F_{i_{o\,\text{at (V)}}}}{\Delta V}\right] = r_i$$

Now taking the limit ΔV→0

$$\Rightarrow \quad \lim \Delta V \to 0 \left[\frac{F_{i \text{ at } (V+\Delta V)} - F_{i_{o\,\text{at (V)}}}}{\Delta V}\right] = r_i$$

$$\Rightarrow \qquad \left[\frac{d\,F_i}{dV}\right] = r_i$$

This is required differential form of performance equation for plug flow reactor.

Now this at time t usually is used for the measurement of a performance in the batch reactor. Similarly, space time and space velocity they are used as the performance measure in any kind of flow system within the reactor system. Now space time, this is the time required for processing of one reactor volume of feed in a flow reactor at some specified temperature and pressure and other conditions of the reaction.

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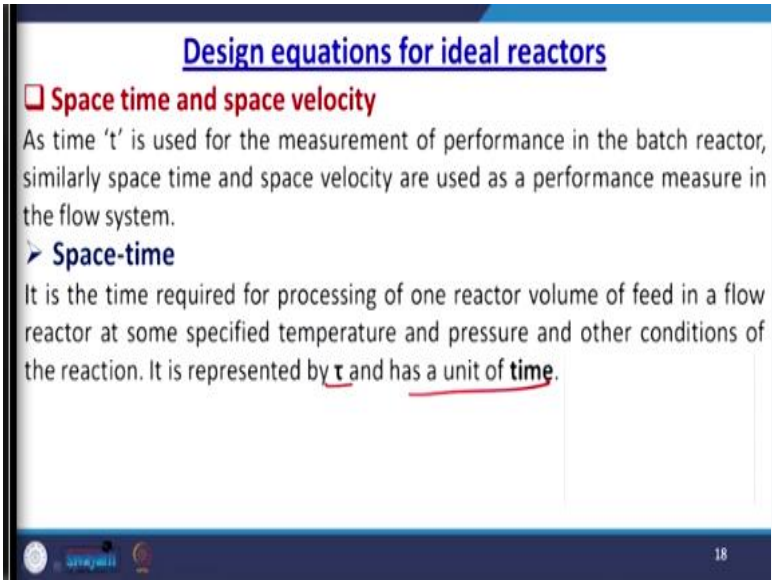

Design equations for ideal reactors

❑ **Space time and space velocity**

As time 't' is used for the measurement of performance in the batch reactor, similarly space time and space velocity are used as a performance measure in the flow system.

➢ **Space-time**

It is the time required for processing of one reactor volume of feed in a flow reactor at some specified temperature and pressure and other conditions of the reaction. It is represented by τ and has a unit of **time**.

Now it is usually represented as tau and has a unit of time. Now mathematically if we wish to represent this space time.

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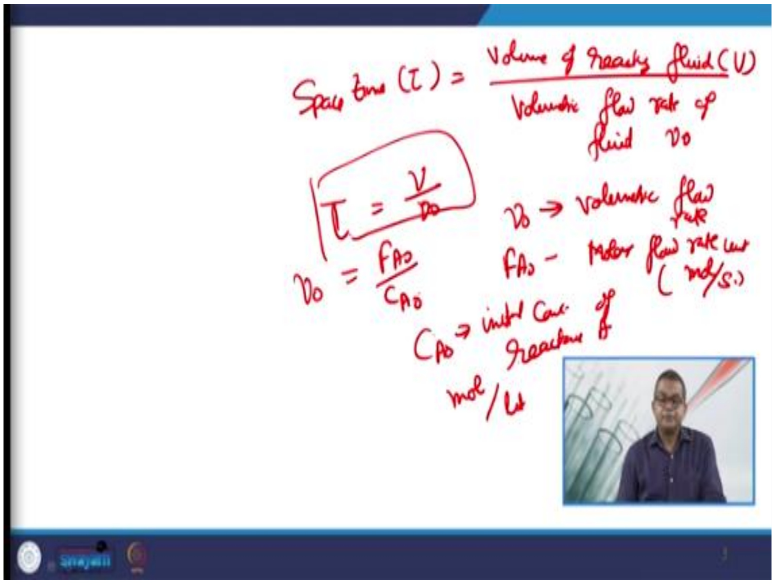

Space time $(\tau) = \frac{\text{Volume of reacting fluid } (V)}{\text{Volumetric flow rate of fluid } v_0}$

$\boxed{\tau = \frac{V}{v_0}}$

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

$v_0 \rightarrow$ volumetric flow rate

F_{A0} – Molar flow rate unit (mol/s)

$C_{A0} \Rightarrow$ initial conc. of reactant A mol/lit

This is space time tau = volume of reacting fluid that is V divided by volumetric flow rate of fluid. So, tau is equal to and here this nu 0 = F_{A0} upon c, now this is the volumetric flow rate this is equal to molar flow rate unit and represented as mole per second. And C_{A0} is the initial concentration of reactant A, having the unit of mole per liter.

It is represented by τ and has a unit of time.

$$\text{space time } (\tau) = \frac{\text{(volume of reacting fluid) V}}{\text{(volumetric flow rate of fluid) } \nu_o}$$

$$\tau = \frac{V}{\nu_o}$$

$$\nu_o = \frac{F_{A_o}}{C_{A_o}}$$

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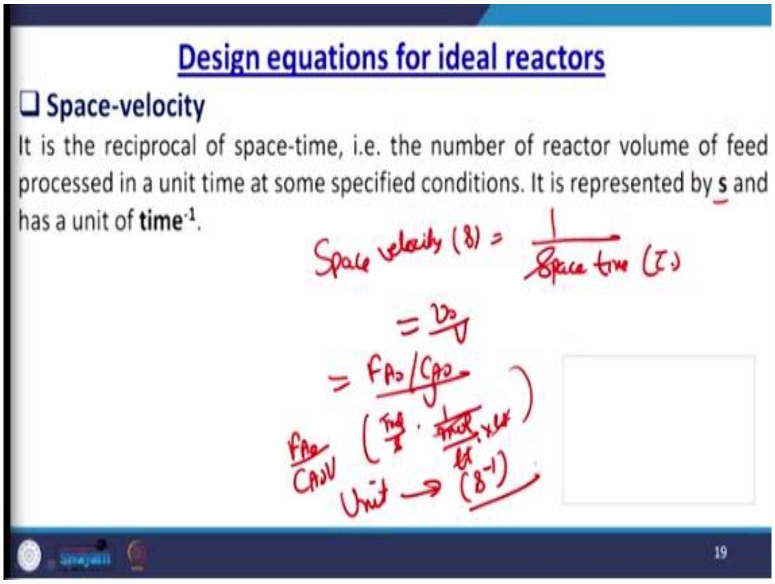

Design equations for ideal reactors

☐ **Space-velocity**

It is the reciprocal of space-time, i.e. the number of reactor volume of feed processed in a unit time at some specified conditions. It is represented by **s** and has a unit of **time^{-1}**.

$$\text{Space velocity } (s) = \frac{1}{\text{Space time } (\tau)}$$

$$= \frac{\nu_0}{V}$$

$$= \frac{F_{A0}/C_{A0}}{V}$$

$$\frac{F_{A0}}{C_{A0}V} \quad ([illegible])$$

Unit → (s^{-1})

Now another good concept is the space velocity, this is usually the reciprocal of space time that is the number of reactor volume of feed processed in unit time at some specified conditions may be related to the pressure, temperature etc. And it is represented by small s and has the unit of time inverse. So, mathematically we can put forward like this space velocity, space time or F_{A0}, so unit is second inverse, so this is the space velocity.

$$\text{Space velocity } (s) = \frac{1}{\text{space time } (\tau)} = \frac{\nu_o}{\text{V}} = \frac{\left(\frac{F_{A_o}}{C_{A_o}}\right)}{V}$$

Now space time sorry now in general way we can say that if there is a space time of say 5 hours for a reaction to complete. Then it means that there is 5 hours required to process one reactor volume feed. And if we say that the space velocity is given by 5 hours inverse, that is 5 reactor volumes are processed in an hour under the specified conditions of the reaction with respect to the temperature and pressure.

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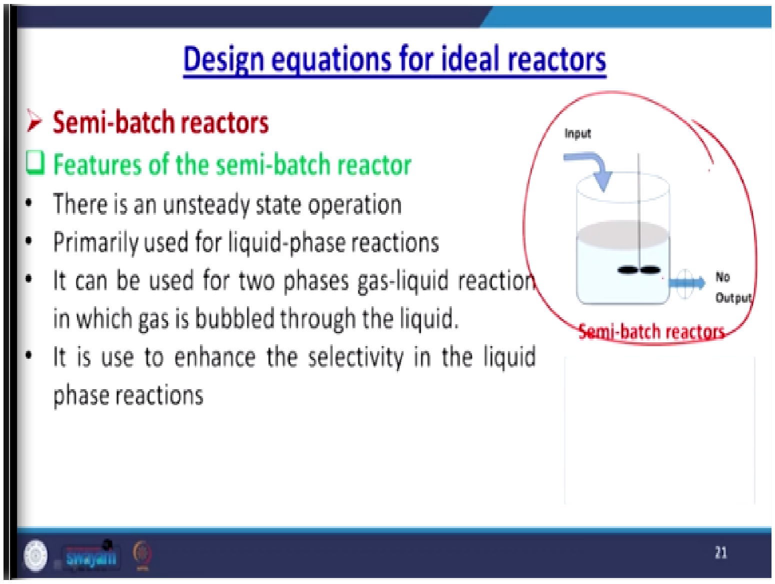

Design equations for ideal reactors

- Semi-batch reactors

☐ Features of the semi-batch reactor

- There is an unsteady state operation
- Primarily used for liquid-phase reactions
- It can be used for two phases gas-liquid reaction in which gas is bubbled through the liquid.
- It is use to enhance the selectivity in the liquid phase reactions

Now let us have a consideration of semi batch reactor. Usually there are various features associated with the semi batch reactor. As you see that here in the figure there is an input and usually output is restricted. So, this is an unsteady state type of operation and primarily being used for various liquid phase reactions. So, it can be used in 2 phases maybe the gas liquid reactions where the gas is usually bubbled or spurged through the liquid.

And it used to enhance the selectivity of liquid phase reaction. Again, there are various advantages and disadvantages associated with this semi batch reactor. Now it has advantages of controlling the reaction rate and temperature. And it has a concept of minimization of unwanted side reaction by maintaining the low concentration of reactants. So, this type of thing you can easily control within this semi batch reactor.

There are couple of disadvantages within the semi batch reactor, that it again requires the higher labor cost for charging, discharging cleaning per batch etc. There is a variation in the product quality per batch because it all depends on a batch type of the scenario. Therefore, in based on these two disadvantages and couple of advantages associated with it is best suited for small scale industrial operation.

Now let us have look about the different type of semi batch reactor. There are 2 type of semi batch reactor, usually they are used to enhance the selectivity in the liquid phase reaction.

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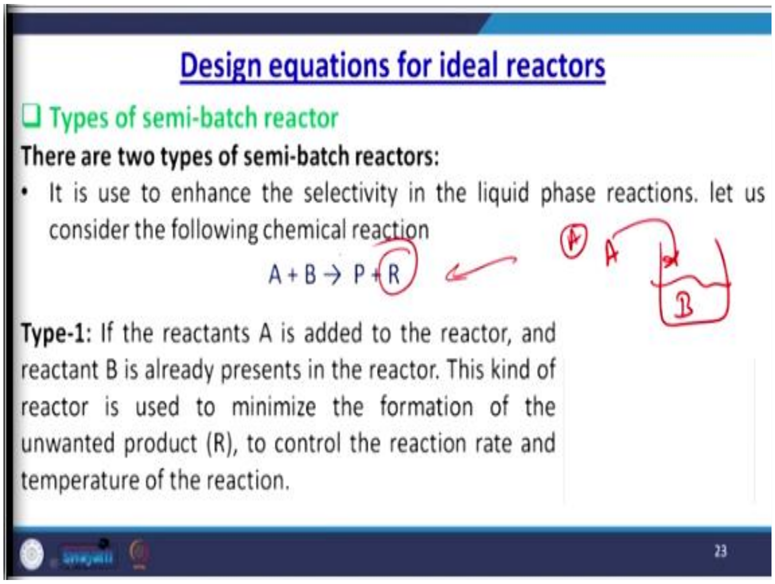

Design equations for ideal reactors

☐ Types of semi-batch reactor

There are two types of semi-batch reactors:

- It is use to enhance the selectivity in the liquid phase reactions. let us consider the following chemical reaction

$$A + B \rightarrow P + R$$

Type-1: If the reactants A is added to the reactor, and reactant B is already presents in the reactor. This kind of reactor is used to minimize the formation of the unwanted product (R), to control the reaction rate and temperature of the reaction.

So, let us consider this particular general chemical equation which we discussed priorly A + B = P + R. So, the type 1, if reactant A is added to the reactor and B is already present in the reactor. So, this kind of a reactor just gave a figurative approach B is present and you are adding A into it. So, this kind of reactor is used to minimize the formation of any kind of unwanted product sometimes maybe referred as R to control the reaction rate and a temperature of the reaction.

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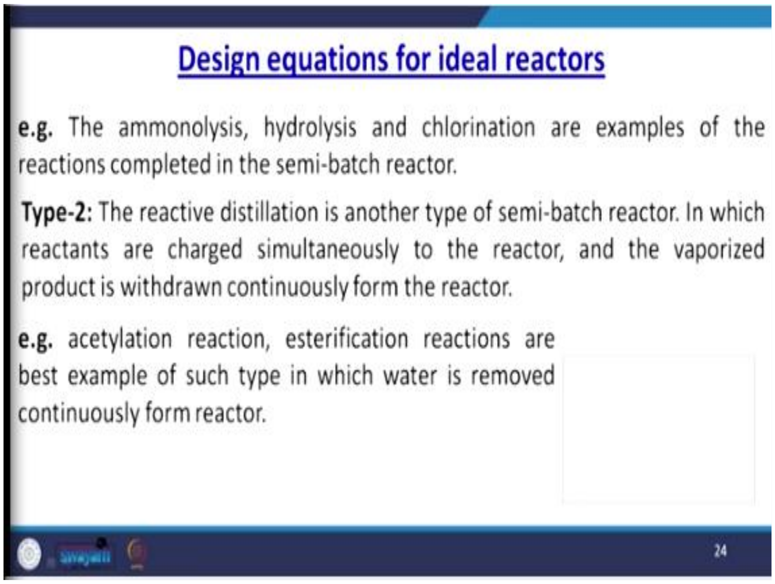

Design equations for ideal reactors

e.g. The ammonolysis, hydrolysis and chlorination are examples of the reactions completed in the semi-batch reactor.

Type-2: The reactive distillation is another type of semi-batch reactor. In which reactants are charged simultaneously to the reactor, and the vaporized product is withdrawn continuously form the reactor.

e.g. acetylation reaction, esterification reactions are best example of such type in which water is removed continuously form reactor.

Now couple of examples of this particular type of reactor that is ammonolysis, hydrolysis, chlorination etc. Now another type of reactor is that the reactive distillation usually is another type of semi batch reactor in which reactants are charged simultaneously to the reactor. And vaporized product is withdrawn continuously from the reactor, the example of this particular reaction is acetylation reaction, esterification reaction.

They are the best suited example for such type of reactor where water is continuously being removed from the reactor, so that you can maintain the appropriate condition within the reactor. Now let us have a look about the various design equations for the single reacting system under the batch reactor.

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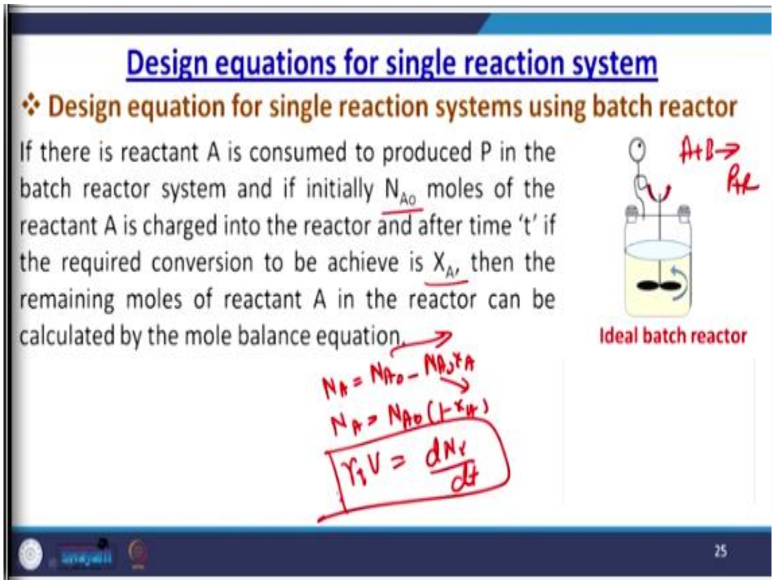

Design equations for single reaction system

- Design equation for single reaction systems using batch reactor

If there is reactant A is consumed to produced P in the batch reactor system and if initially N_{A0} moles of the reactant A is charged into the reactor and after time 't' if the required conversion to be achieve is X_A, then the remaining moles of reactant A in the reactor can be calculated by the mole balance equation.

$A + B \rightarrow P + R$

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

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

$\boxed{r_A V = \frac{dN_A}{dt}}$

25

Now if there is a reactant A in consumed to produce P in the previous equation. And initially if say that N_{A0} moles of the reactant A is charged into the reactor. Say after some time t, if the required conversion to be achieved and this may be referred as X_A then the remaining mole of reactant A in the reactor it can be calculated by the basic mole balance equation and that is $N_A = N_{A0} - N_{A0} X_A$.

Now here this N_{A0} is the initial number of moles of A and this $N_{A0} X_A$ moles of A consumed within the reaction. So, this equation can be represented as $1 - X_A$ and the differential performance equation for this ideal batch reactor can be represented like this.

Moles of reactant A remaining $(N_A) = N_{Ao}(1 - X_A)$

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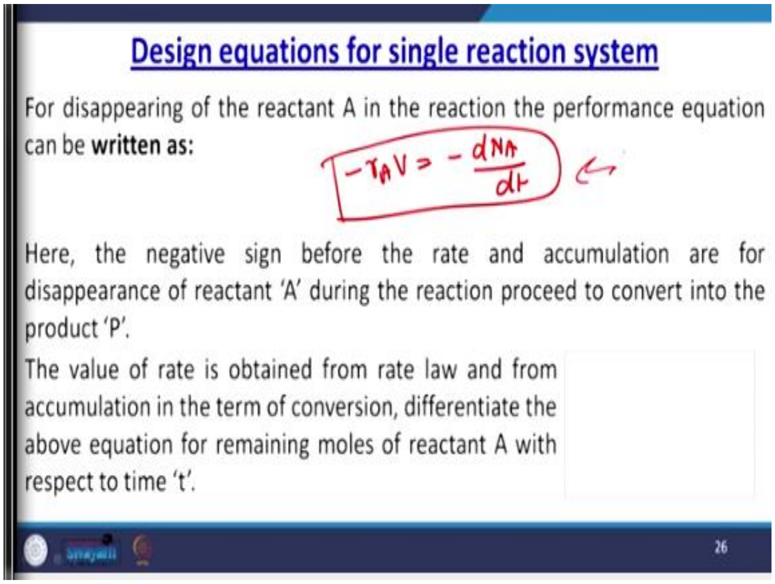

Design equations for single reaction system

For disappearing of the reactant A in the reaction the performance equation can be **written as:**

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

Here, the negative sign before the rate and accumulation are for disappearance of reactant 'A' during the reaction proceed to convert into the product 'P'.

The value of rate is obtained from rate law and from accumulation in the term of conversion, differentiate the above equation for remaining moles of reactant A with respect to time 't'.

Now for disappearing of reactant A in the reaction the performance equation we can write like this. Now here the negative sign before the rate of and accumulation or for the disappearance of reactant A as I discussed previously. During the reaction proceeds and this convert into the product P. So, the value of rate is obtained from the rate law and from accumulation in term of conversion differentiate the above equation this equation for remaining moles of reactant A with respect to time.

The differential form of performance equation for ideal batch reactor is given as

$$r_i V = \frac{dN_i}{dt}$$

For disappearing of the reactant 'A' in the reaction the performance equation can be written as

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

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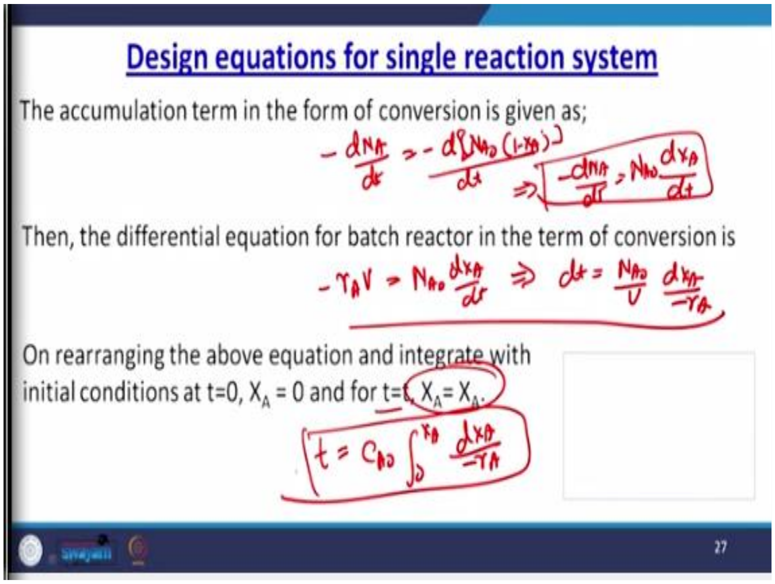

Design equations for single reaction system

The accumulation term in the form of conversion is given as;

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

Then, the differential equation for batch reactor in the term of conversion is

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

On rearranging the above equation and integrate with initial conditions at t=0, $X_A = 0$ and for t=t, $X_A = X_A$.

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

Now accumulation, if we talk about the accumulation, accumulation term in the form of conversion is given as - dN_A and dt or. Now then the differential equation for the batch reactor in terms of conversion can be written as - r_A $N_{A0}X_A$ dt. Now if we integrate with and rearrange the things keeping in an i over the initial conditions at t = 0. And at this point $X_A = 0$ and for t = t and this point the X_A = X, then we can represent like this; now this is we can say the required performance equation for batch reactor at constant time. Now sometimes you need to put the graphical representation of performance equation for the batch reactor.

Then, the differential equation for batch reactor in the term of conversion is

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

On rearranging the above equation and integrate with initial conditions at t=0, $X_A = 0$ and for t=t, $X_A = X_A$.

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

This is the required performance equation for batch reactor for constant volume reactor system.

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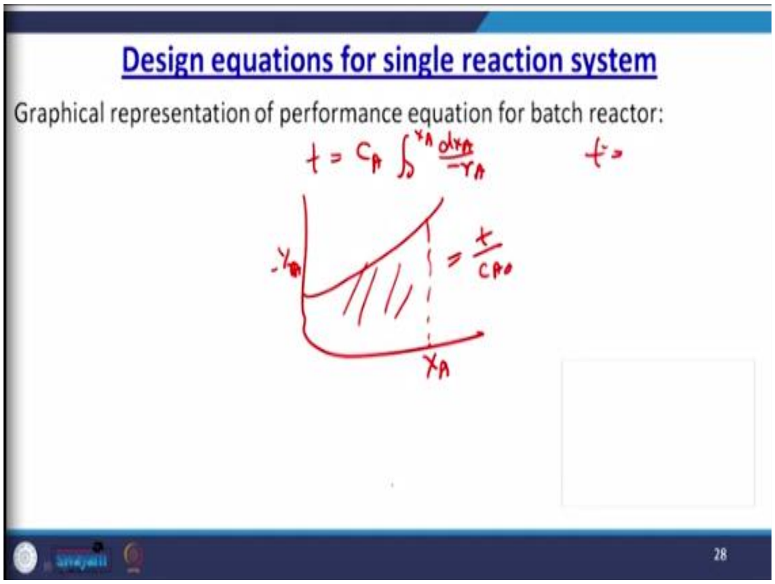

Design equations for single reaction system

Graphical representation of performance equation for batch reactor:

$t = C_A \int_0^{X_A} \frac{dX_A}{-r_A}$ $t =$

And the governing equation for this one is and t is now if you wish to plot the things. This is X_A and this is 1 upon r_A is very common thing. Now this area under this particular curve like this = t upon C_{A0}.

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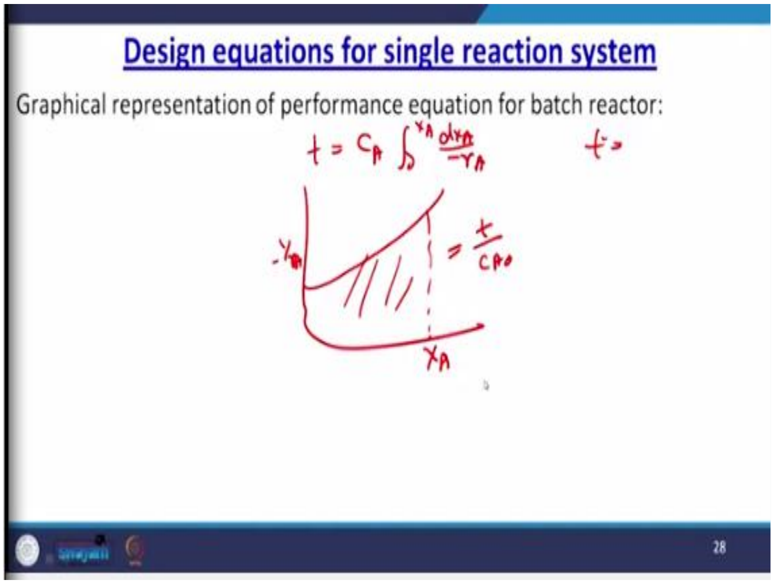

Design equations for single reaction system

Graphical representation of performance equation for batch reactor:

$t = C_A \int_0^{X_A} \frac{dX_A}{-r_A}$ $t =$

Similarly, if I go for 1 upon r_A versus C_A, now here this is the C_{A0}, now the governing equation for this particular type of scenario is your C - r_A. So, by this way you can predict the situation; now for varying volume system if we putting the varying volume relation in the rate law, the performance equation we can write like this.

$$-r_A V_o(1+\varepsilon_A X_A) = N_{A_o}\frac{dX_A}{dt}$$

$$\int_0^t dt = N_{A_o}\int_0^{X_A}\frac{dX_A}{V_o(1+\varepsilon_A X_A)(-r_A)}$$

$$\Rightarrow t = N_{A_o}\int_0^{X_A}\frac{dX_A}{-r_A V_o(1+\varepsilon_A X_A)}$$

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

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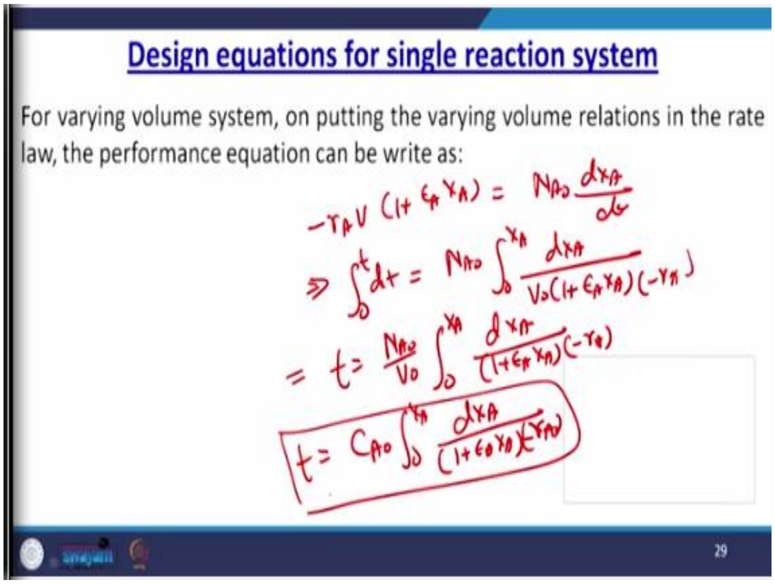

Design equations for single reaction system

For varying volume system, on putting the varying volume relations in the rate law, the performance equation can be write as:

$$-r_A V(1+\varepsilon_A X_A) = N_{A0}\frac{dX_A}{dt}$$

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

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

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

Now something for if you recall the previous plot N_{A0} this is t = N_{A0} upon V_0 0 to X_A because t = 0 and X_A = x then d X_A upon 1 + epsilon A X_A and 2 - r_A or t can be represented as C_{A0} 1 + epsilon A X_A - r_A. So, this is your performance equati`on for this particular situation.

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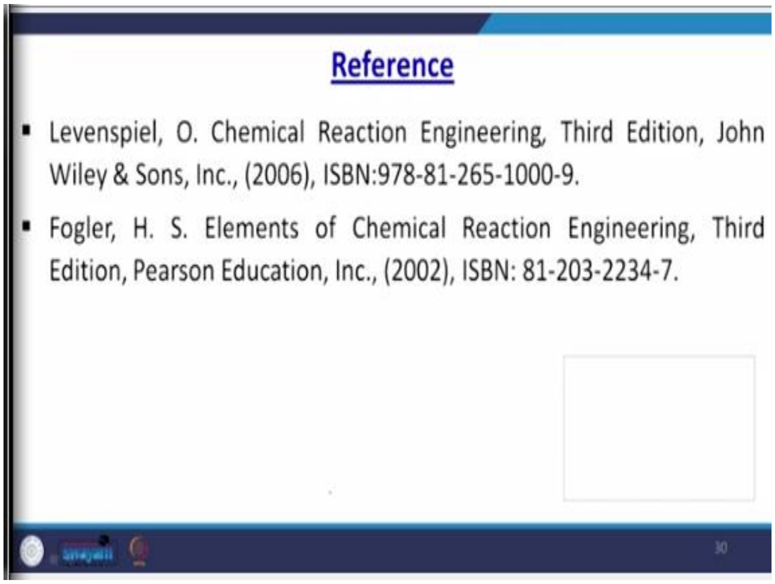

Reference

- Levenspiel, O. Chemical Reaction Engineering, Third Edition, John Wiley & Sons, Inc., (2006), ISBN:978-81-265-1000-9.
- Fogler, H. S. Elements of Chemical Reaction Engineering, Third Edition, Pearson Education, Inc., (2002), ISBN: 81-203-2234-7.

Now in this particular lecture we discussed about the various design equations for various kind of reaction system. And we developed various performance equation attributed to all kind of reacting system. Now if you wish to have further reading related to these particular concepts, you can have a look of these references which are enlisted in this particular slide, by this way thank you very much.