Polymer Reaction Engineering
Prof. Shishir Sinha
Department of Chemical Engineering
Indian Institute of Technology - Roorkee

Lecture – 12
Introduction to Reactor Design - I

Welcome to the new lecture of introduction to reactor design. Now earlier during the course of this polymer reaction engineering, we studied about what are the polymerization process, what are the different classifications associated with the polymerization reaction, what are the different governing factors they attribute to the property of the polymers? And we see that the molecular weight distribution, temperature, catalyst, etc., they play a very vital role while deciding the properties of the polymer.

So, based on this thing where you need to carry out the polymerization process that is a place called reactor. And the proper designing of a reactor is very essential to control various properties of polymerization process because you see that all these properties are very sensitive in nature. A slight variation in either the flow property of say initiator or particle size controller or temperature, etc. they may create a severe problem during the course of reaction.

Sometimes mass may become so bulky, viscosity may become so large so that you cannot further process the reactor. So slight variation may cause a bit difficulty. One best example is that if you vary the quantity or the concentration of particle size controller in polystyrene divinylbenzene bead preparation, then it may create a severe problem and the entire mass will get destroyed over the period of time.

So, it adversely affects the economics energy consideration of the particular process. So, based on this particular criterion and based on the desireness of the polymer properties, this particular chapter gives you a brief outline that how you can go ahead with the different parameter control through the reactor design.

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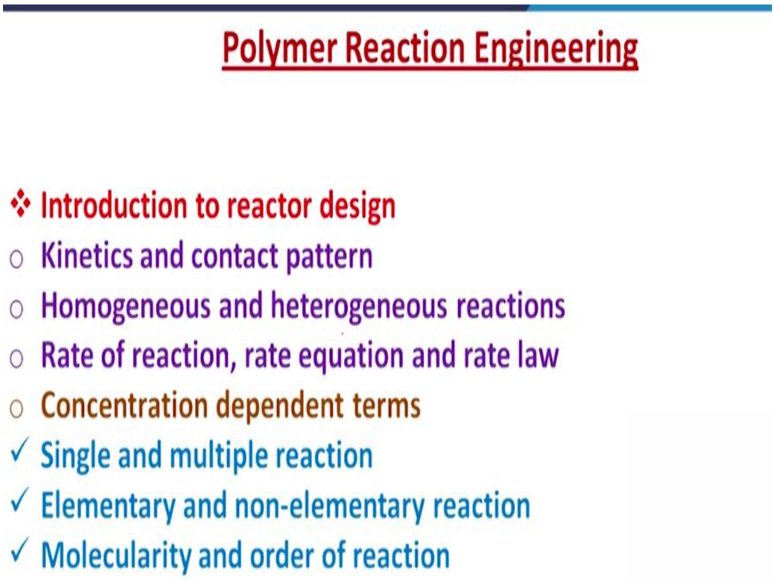

Now there are some segments of this particular lecture or chapter. They are the introduction to reactor design where we will discuss that what is the efficacy of the reactor. Then we will discuss about the kinetic and contact pattern of all kind of reactors. We will discuss about the homogeneous and heterogeneous reactions because the variety of the polymerization process triggers this particular approach.

Then we will discuss about the rate of a reaction, what kind of the different rate equations? What are the governing factors? What are the different rate laws attributed to all these polymerization process? We will have concentration dependence term discussion over the period of time which will discuss about the single or multiple reactions. We will have a discussion about the elementary and non-elementary reactions, molecularity and order of the reaction.

All these things play a very vital role while deciding the approaches of polymerization process and slight variation or slight disturbance in all kind of approach may create the polymerization process to the negative direction whatever you desire.

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Introduction to Reactor Design

❖ Reactor Design

There are needs of knowledge, experiences and information required from different areas such as chemical kinetics, fluid mechanics, heat transfer, thermodynamics, mass transfer and economics etc. to design a reactor.

- ✓ To produced a desired product industrially, there are needs of physical treatment (separation, purification) of the raw material in the form in which they react chemically and then they pass through the reactor.

So, let us have a look about the concept of reactor design. Now there are needs of knowledge, experience and information they require from different area such as chemical kinetics, fluid mechanics, heat transfer, thermodynamic approach, mass transfer, economics, etc. to design a reactor. Just I am giving an example like in the previous lectures we studied about the flow pattern of the various constituents those who are participating in the polymerization reaction.

We discussed a lot about the exothermicity and endothermicity of all those polymerization reactions in due course of time. And we discussed that all these parameters play a very vital role in the ultimate properties of the polymers. So, these types of things you need to control within the reactor, and you need to give a due importance to all these factors. Now the ultimate aim if you see that is to produce the desired product industry.

Now for there is a need to make all these things under the head of a physical treatment that is the separation purification of the raw material in the form in which they react chemically and then they pass through the reactor. Now there are other complicacy in the reactor design that obviously all the reactants which we are introducing in a particular reactor pattern, they do not participate in the reaction mass 100%.

So, you need to separate and if you see that in the condensation or the polymerization process in that process you need to extract the byproduct from the reaction mass. So, you need to encounter these kinds of a separation problem, sometimes you need to encounter the problem of a purification aspect. So, you need to take all those things into consideration while designing the proper chemical reactor or proper polymerization reactor.

And above all slight variation may cause a problem of economic approach. If your reaction destroys, then definitely the loss to the industry, loss to the economic on the adverse side. So, keeping in view of all these factors you need to take the things in in a very sensitive manner. Now sometimes the question arises that what kind of information you require to predict the efficacy or working style of the reactor?

In broad spectrum, we may have two three different points which may be very helpful while designing the reactor.

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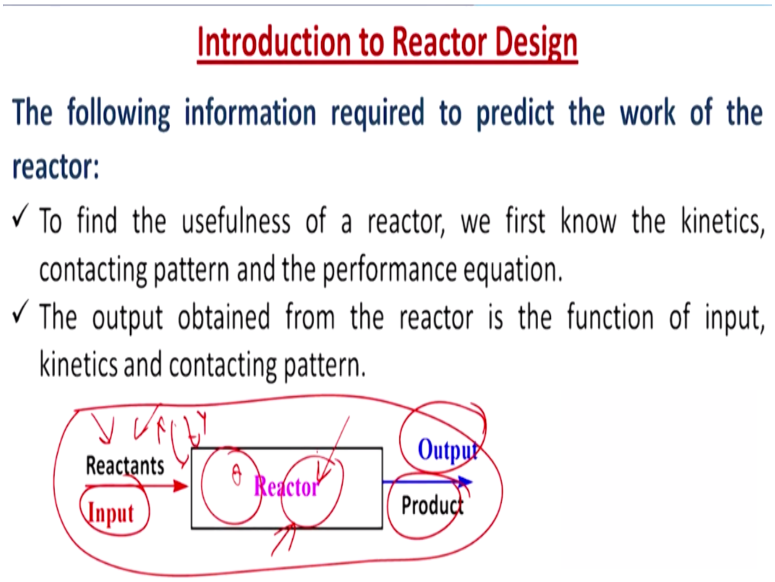

One is that to find the usefulness of a reactor. So, in this approach we should know that the kinetic contacting pattern and the performance equation. These are the very common phenomena of any kind of a reaction engineering approach. Second thing is that the output obtained from the reactor usually is a function of input kinetics and contacting pattern. Now you see this is a generalized diagram of any kind of a reactor.

Here you are putting the reactor as an input stream and here you are getting the product as an output stream. Now just you see that this is a very simple reactor. Now when we talk about this particular thing, we should know that what is happening inside? What is the purity of my reactants? How much they are participating in this particular reactor? What is the fate of the unreacted stream? How are you separating any kind of the byproduct being generated?

How you are separating the product which is desired from the reaction mass? How are you controlling the properties of the product? So, all these factors you need to take into consideration while deciding the fate or while designing the reactor in any course.

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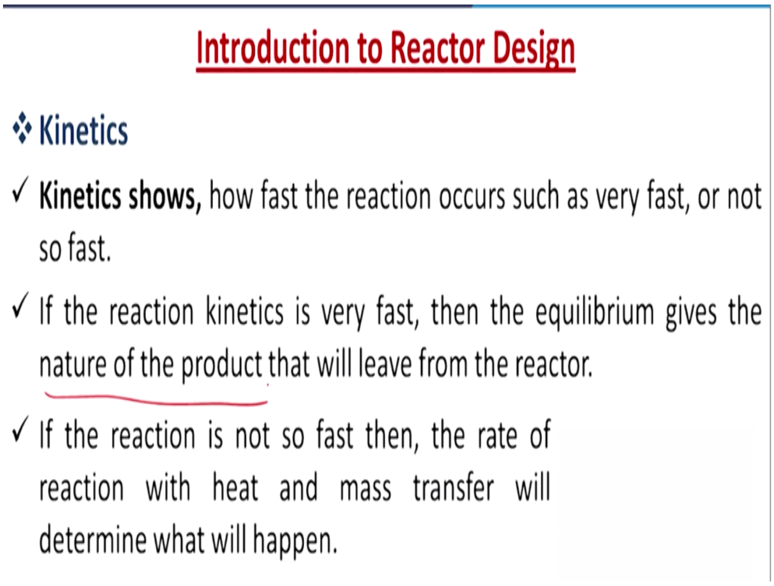

Now to help in this approach, kinetics plays a very vital role. This shows that how fast the reaction occurs such as very fast or not so fast. Now again these two approaches, let me give you a brief outline about that what are these approaches. Now if the reaction kinetic is very fast, then sometimes equilibrium gives the nature of the product that will leave from the reactor. So ultimate aim is to get that acquaintance with the nature of the product.

Now sometimes if the reaction is not so fast, then the rate of reaction with heat and mass transfer will determine what will happen. Sometimes the feasibility may not be there, sometime conversion may not be there, sometimes yield will not be up to the mark. So, you need to look into all these approaches. Now while we were discussing about this particular reactor now if there are two reactants within this reactor stream say X and Y.

And if they are coming to this particular reactor, then the foremost important thing is that you need to look into that what is the contacting pattern. Let us have a brief look about the contacting pattern.

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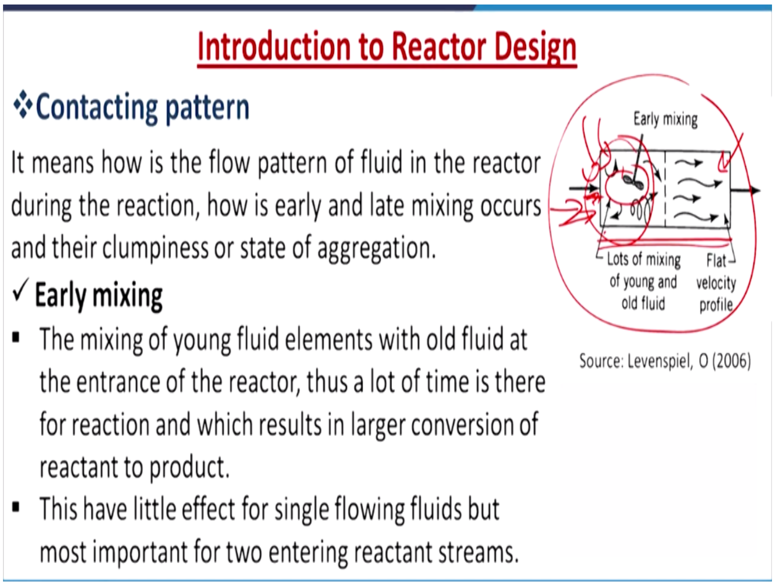

It means that how the flow pattern of fluid in the reactor during the reaction. Now this fluid may be your reactants, this fluid may be the combination of the reactant by product and the product stream. So, this thing should be in your mind and how is early and late mixing occur and their clumpiness or the state of aggression. Let me give you a couple of examples which are related to the early mixing or late mixing, etc. or clumpiness.

Now early mixing; the mixing of young fluid. Now let us see that this particular example from the generalized group. Here this is the input stream. Now the mixing of young fluid that means you are introducing, now if you recall that in the previous lectures we discussed about the batch, semi batch and a continuous reactor. So, the mixing the of young fluid element with old fluid one at the entrance of the reactor.

Here you see that this is the entrance of the reactor and the fluid which is coming inside to the reactor is having the intimate contact with the old fluid. So, a lot of time is there for the reaction which results in the larger conversion of the reactant to produce or to product. See here you are introducing the reactants, suppose this is the length of your reactor now in that case you may have you may experience a larger time of reaction.

Now this will have a little effect or a single flowing fluid but most important is for the two entering reactant streams. Just I gave you that if two entering reactant streams, then it may create a good result in due course of time. So, this is something like this and sometimes during the course of time you may achieve the flat velocity profile because of the tendency in the mixing pattern.

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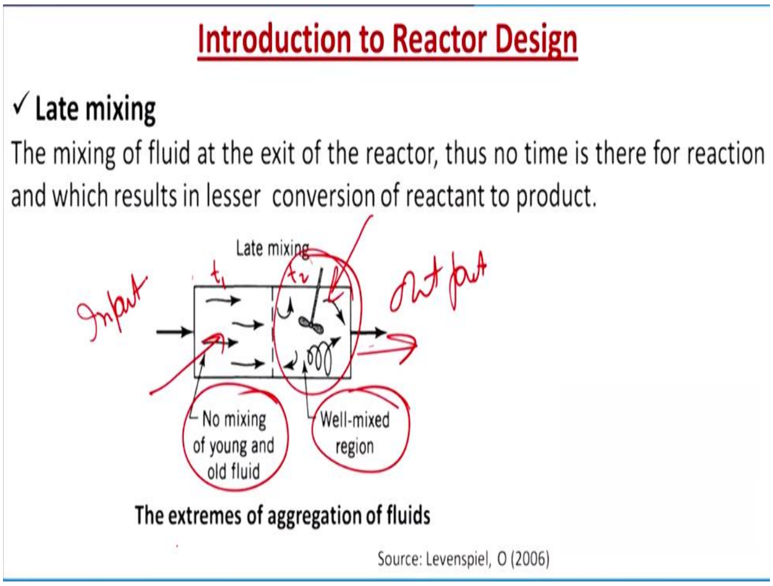

Now there is another concept that is called the late mixing. Now this is the mixing of a fluid at the exit of the reactor. You see here this is the input stream and here you are having the output stream. So here this is at the output of the reactor you are mixing of the fluid. Therefore, you may experience less time for the reaction, and which may result in lesser conversion of reactant to product.

So, you are introducing the things over here or this is sometimes you can say the well-mixed region and here you may experience no mixing or etc. Or sometimes if you are not introducing any reactant or any stream at this juncture and sometimes you are over the period of time say t after t1, you start the late mixing at time t2. So, this gives you a proper agitation and a proper mixing so that the conversion may achieve a bit you can say on the higher side.

But the time consumption for this particular mixing is on the lower side. So, this is the extremes of the aggregation of a fluid.

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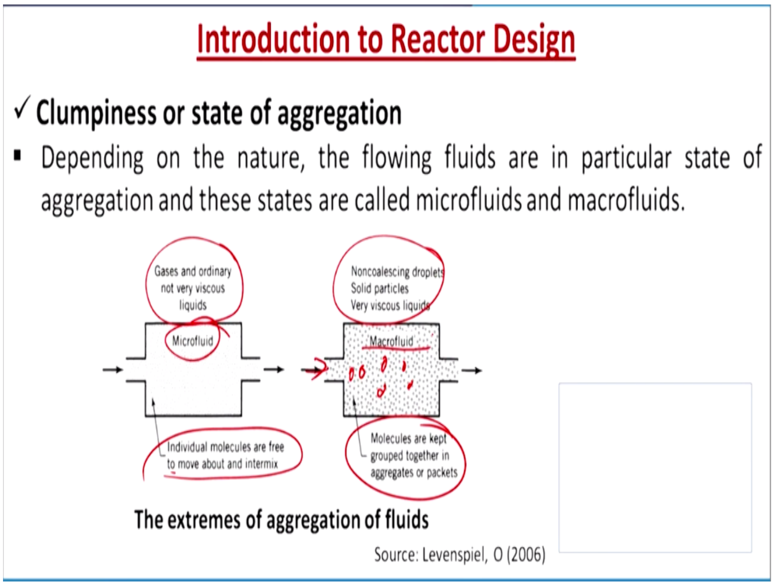

Now sometimes you may experience the state of clumpiness or sometimes that is referred as state of aggregation. Now this depends on the nature of the fluid flow in a particular state of aggregation and these states are called the microfluids or macrofluids. Now here you see in this particular figure, this is the gas and ordinary system which are not very viscous in nature and they are introduced and you may experience that individual molecules are free to move.

And sometimes you may see the intermixing of all these molecules. Now here in this particular figure, so this is the approach of microfluid. Now here there are noncoalescing droplets of solid particles and sometimes you may have a viscous or a very viscous liquid in due course of time. And sometimes you may experience that molecules are kept grouped like this together in aggregates or packets.

And sometimes forms this type of aggregate so they may join over there. So, they may form the situation of macrofluids. So, this is again one criterion and you can say one governing factor while we are designing the reactor for a particular polymerization process.

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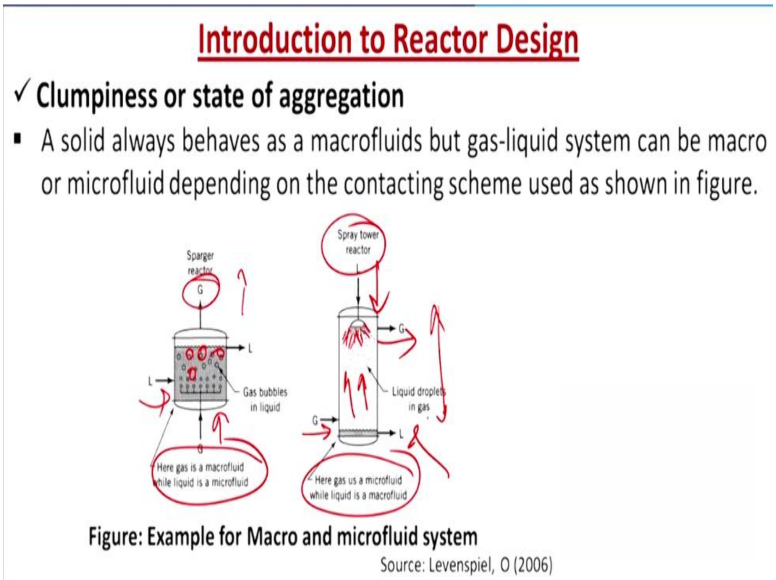

Now usually when solid always behaves as a macrofluid, but a gas liquid system they can be a macro or a microfluid. This depends on the contacting scheme like we have shown you that this particular contacting scheme. Now here the gas is a macrofluid while we are introducing the liquid is the microfluid. So, you are creating the sparger system over here. So, all these gas bubbles they are having the intimate contact with the liquid phase.

And whatever gas even if there is a reaction, so if any kind of a left-over gas may discharge from this particular pore. So here the gas is macrofluid and while liquid is a microfluid. Now here you see that this is the spray tower and its again very common you know industrial phenomena and if you need to produce some spherical particles this particular phenomenon is quite useful. So here this is the spray tower.

Here you are pumping the liquid and here you are spraying the things to the entire reactor and whatever liquid droplets are there they are having the intimate contact with the upward direction moving gas or system. So, you may have the intimate contact of liquid with the gaseous system. So here gas is a microfluid and liquid is a macrofluid. So, these type of various clumpiness or state of aggregation are very common and applicable in the industrial application in due course of time.

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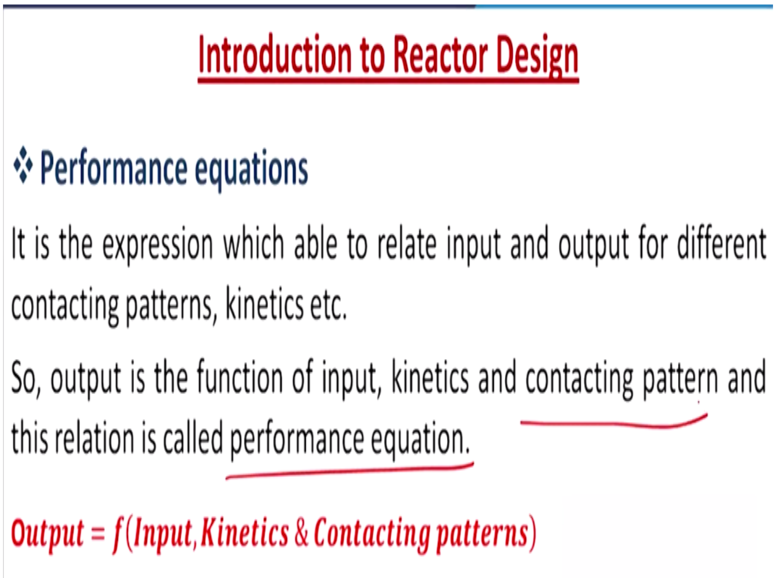

Now another important factor which we should know about the performance equation. This is again a very important aspect related to the reactor design. Now it is the expression which appears to relate input and output of different contacting pattern, kinetics, etc. because see you are having different variables, so you need to have an expression or a mathematical correlation through which you relate all those things under the head of output.

$$Output = f(Input, Kinetic \; \& \; Contacting \; patterns)$$

Because your ultimate aim is to decide the properties and to have a fixed property of or desired property of your output stream. So output is usually the function of input stream whatever the concentration of your raw material, whatever things you are putting inside that reactor, then the kinetics and then the contacting pattern and this relation is called the performance equation. Now see we have already discussed the importance of input stream.

We have already discussed briefly about the importance of the kinetic and then contacting pattern. So, you may refer that the output is a function of input, kinetics and contacting pattern. Trust me this implies a very vast parametric equation which you can input, or you can introduce a different type of a parameters closely associated with your polymerization reaction. Now when we go for the reactor design concept, we must know about the various classification of a reaction.

This will ease out your working credo so that you can pick a proper reactor, you can design the proper reactor for any kind of a polymerization reaction. So, as I told you that these reactions can be classified in either homogeneous or heterogeneous system. So, let us have a look about a brief with respect to the homogeneous reaction. Now if the reaction takes place in a single phase that is all the reactants and products are under the head of a same phase may be liquid or a gas then the reaction is said to be the homogeneous.

And most of the gas phase reactions are fast reactions such as burning of the flame, the example of noncatalytic and homogeneous reaction. Whereas most of the liquid phase reactions are again called the homogeneous reaction and they are the catalytic reaction. So, you may have subclassification among this particular head that is noncatalytic homogeneous reaction and catalytic homogeneous reaction.

Then go back to this heterogeneous reaction, now this reaction which requires at least two phases to proceed at the end of the product formation and such type of reactions are heterogeneous in nature. So, most of the gas phase reactions such as burning of coal, gas liquid absorption with the reaction they are noncatalytic type of heterogeneous reaction. And oxidation of say SO_2 to SO_3 and ammonia synthesis they are the best example of catalytic heterogeneous reaction.

So again, you subclassify these heterogeneous reactions in two heads. One is noncatalytic type of heterogeneous reaction, another one is the catalytic type of heterogeneous reaction. So, this particular information is extremely useful while designing the reactors.

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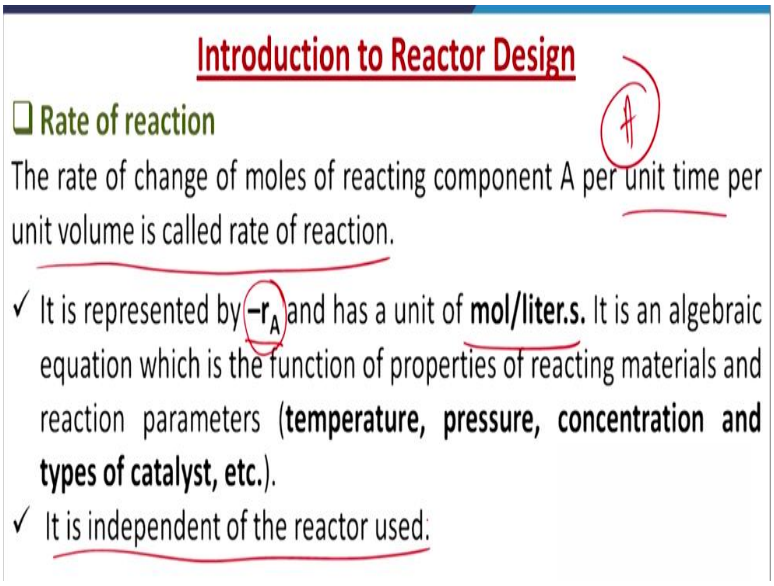

Then another approach is extremely important and that is called the rate of a reaction, and in other words you can say this rate of reaction is the most important part of your reactor design. So, the rate of change of moles of reacting components, let us have two components in the reaction mass. Let us say one is A. So, the rate of change of a moles of a reacting component A per unit time per unit volume is called the rate of reaction.

This is a very broad or a generalized equation. Now usually this is represented by $-r_A$, minus sign just tells you that the moles of A are being consumed in due course of time with respect to the formation of product. So, it is represented as minus $-r_A$ and it has the unit of moles per liter second. And it is an algebraic equation which is usually the function of a properties of reacting material and reaction parameters.

Now the reaction parameters are a different type like temperature, pressure, concentration, type of catalyst and so on. Now this is independent of reactor used but it is a very important factor for the reactor design. So, you cannot overlook the importance of either reactor or reactor design

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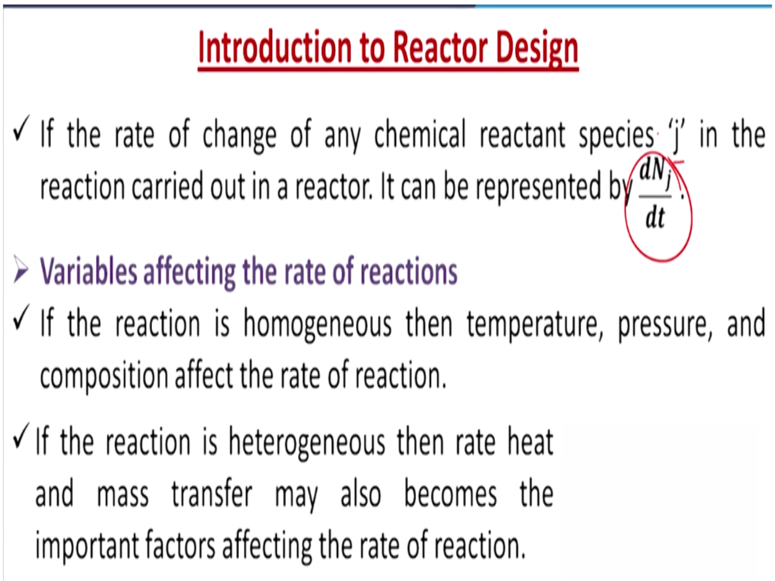

If the rate of change of any chemical reactant especially says j in the reaction carried out in a reactor it can be represented as dN_j by dt, t is time. Now you may ask one question that what are the different variables those who are affecting the rate of reaction? So, if the reaction is homogeneous then temperature, pressure and composition they affect the rate of reaction.

Now if the reaction is heterogeneous then rate heat transfer, mass transfer they may also become the important factor those who are affecting the rate of a reaction. So, these two things must be in mind while designing the reactor attributed to the rate of a reaction. Now let us have about the various classification of rate of reaction. So, the rate of a reaction can be defined in a number of ways which are like based on unit volume of reacting fluids.

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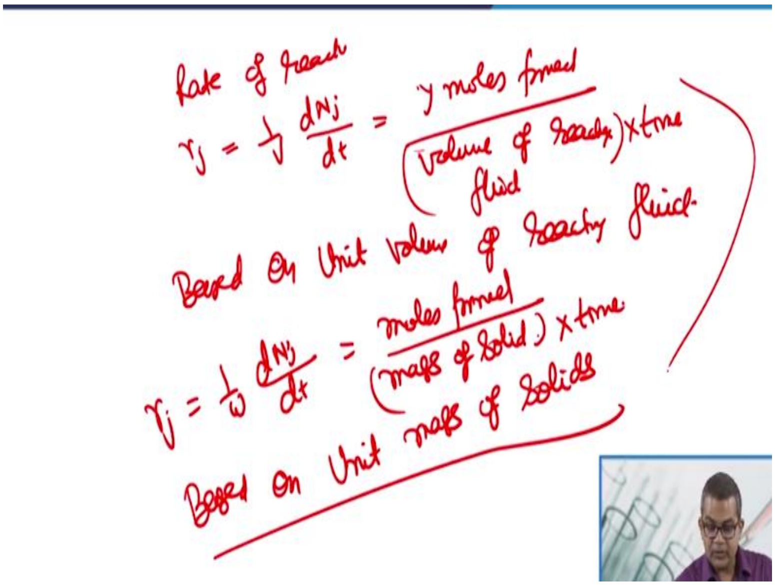

Now this can be represented as rate of reaction, now 1 upon V dNj dt. Now here are the moles formed divided by volume of reacting fluid multiplied by time. Now this is based on unit volume of reacting fluid.

Based on unit volume of reacting fluid

$$r_j = \frac{1}{V}\frac{dN_j}{dt} = \frac{\text{moles of j formed}}{(\text{volume of reactor})(\text{time})}$$

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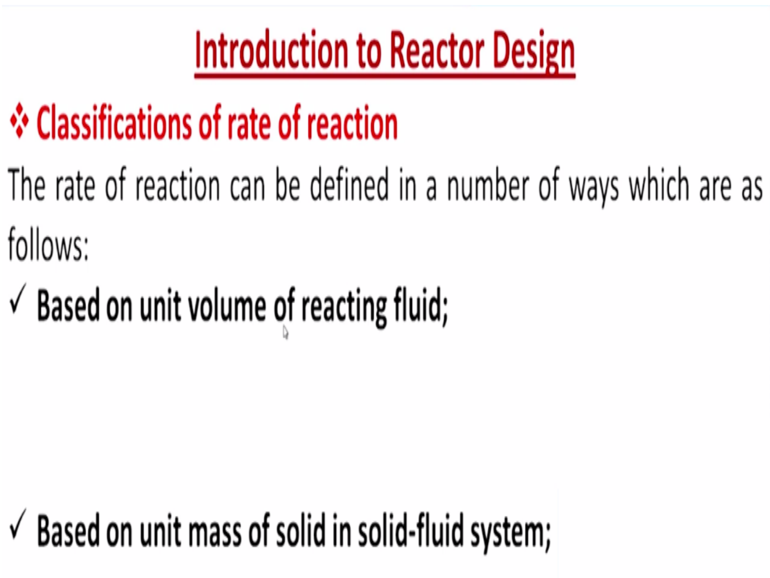

Now if we consider that based on the unit mass of solid in solid liquid system, this is another class of rate of a reaction. Then we can represent as r_j = 1 upon w dN_j upon dt that is the moles formed divided by mass of solid multiplied by time. So, this is based on unit mass of solids. So, these two approaches if you see that the general aspect in these equations are common. This fluid is replaced by solid.

Based on mass of solid in solid-fluid system

$$r_j = \frac{1}{W}\frac{dN_j}{dt} = \frac{\text{moles of j formed}}{(\text{mass of solid})(\text{time})}$$

Another classification is based on the unit interfacial surface in two fluid systems or based on unit surface of solid in a solid gas system.

Based on the unit interfacial surface in the two-fluid system or based on the unit surface of solid in a solid-gas system

$$r_j = \frac{1}{S}\frac{dN_j}{dt} = \frac{\text{moles of j formed}}{(\text{interfacial suface area})(\text{time})}$$

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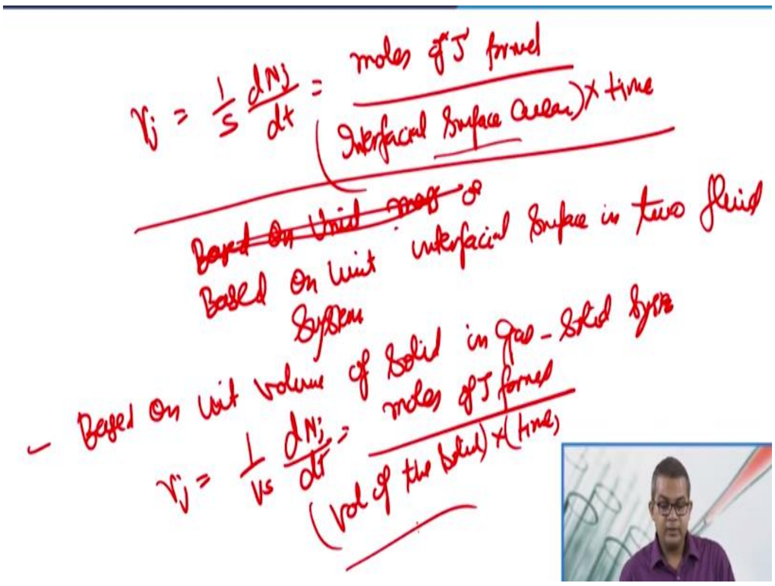

So, let us have a look about this particular mathematical equation this is rate of reaction dN_j that is moles of j formed divided by interfacial surface area into time. So, this is again very important equation. So, this is based on unit interfacial surface in two fluid system.

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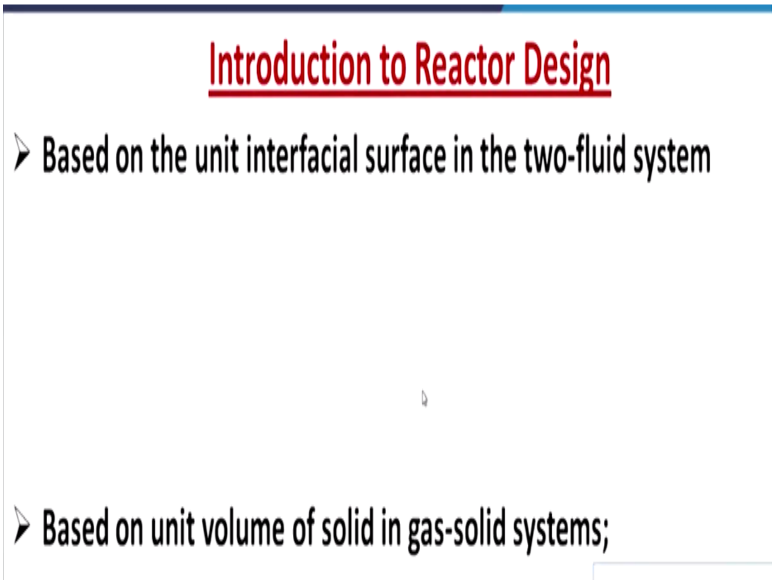

Now another approach is based on unit volume of solid in gas type of a system. Let us have a brief look about the mathematical equation which is attributed to this particular approach that is based on unit volume of solid in gas solid system. This is 1 upon Vs dN_j moles of j formed divided by volume of the solid into time. So, this is again you see that the governing factor is only this one.

Based on unit volume of solid in gas-solid systems

$$r_j = \frac{1}{V_S}\frac{dN_j}{dt} = \frac{\text{moles of j formed}}{(\text{volume of the solid})(\text{time})}$$

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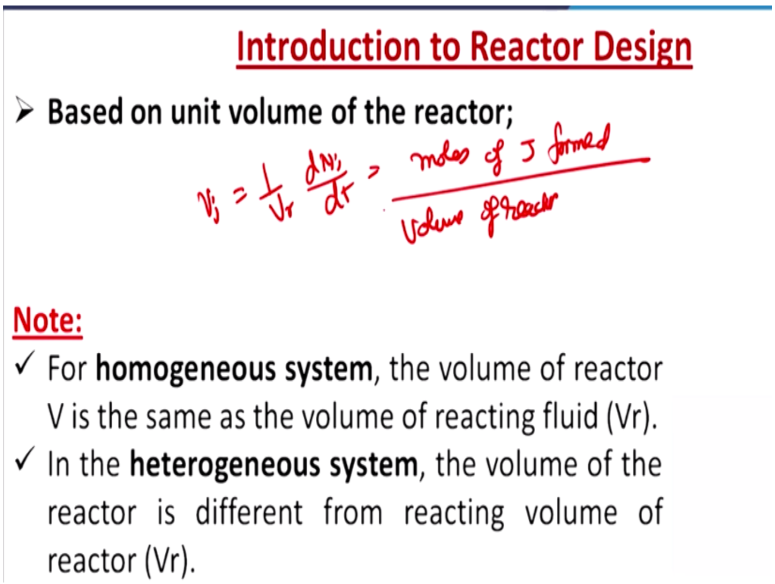

So, another approach is that based on the unit volume of the reactor. Now if you see that this particular equation can be represented at moles of component J formed divided by volume of reactor into time.

Based on unit volume of the reactor

$$r_j = \frac{1}{V_r}\frac{\mathrm{dN}_j}{\mathrm{dt}} = \frac{\text{moles of j formed}}{(\text{volume of the reactor})(\text{time})}$$

So, this is related to the unit volume of the reactor. Now couple of things we should remember while considering all these approaches. Now one is that for homogeneous type of system, the volume of reactor V is same as the volume of a reacting fluid.

This is very important reacting fluid, sometimes it is represented as V_r. Now in heterogeneous system, the volume of the reactor is different from the reacting volume of V_r. So, these two things while designing the reactor should be kept in mind to avoid any kind of confusion related to the reactor design.

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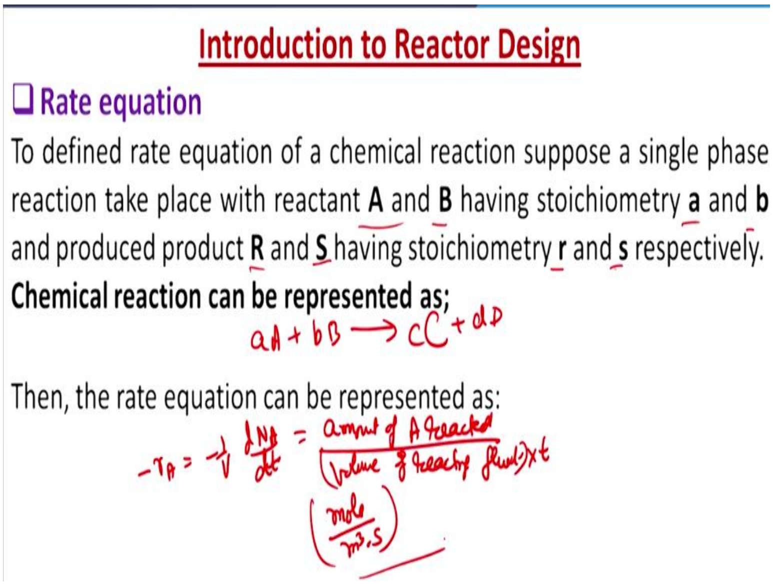

Now let us have a brief look about the rate equation. Now to define the rate of equation of a chemical reaction and this is again very important that suppose a single-phase reaction we are taking into cognizance and there are two reactants A and B those who are having the stoichiometry number small a and small b and products are R and S, again the R and S are having the corresponding stoichiometric number small r and s.

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

So, we can represent the chemical reaction as aA plus capital cC and dD and the rate of a reaction you can write like this. This is for A because see minus sign is put because A is consumed in due course of time. So, –1 upon V dN_A upon dt that is equal to amount of A reacted divided by volume of reacting fluid multiplied by time and the units are mole meter cube second.

The rate equation can be represented as:

$$-r_A = -\frac{1}{V}\frac{dN_A}{dt} = \frac{\text{amount of A reacted}}{(\text{volume of reacting fluid})(\text{time})} \quad \text{in} \left(\frac{\text{mol}}{\text{m}^3.\text{s}}\right)$$

So, this is the rate equation for A and B they both are reacting e to each other for the formation of R and S.

Now another relationship of rate of reaction equation for all the reactant and product with respect to their stoichiometric coefficients if you wish to write now this particular approach is important mathematically because sometimes one may consider, let okay we need to have stoichiometric number into consideration.

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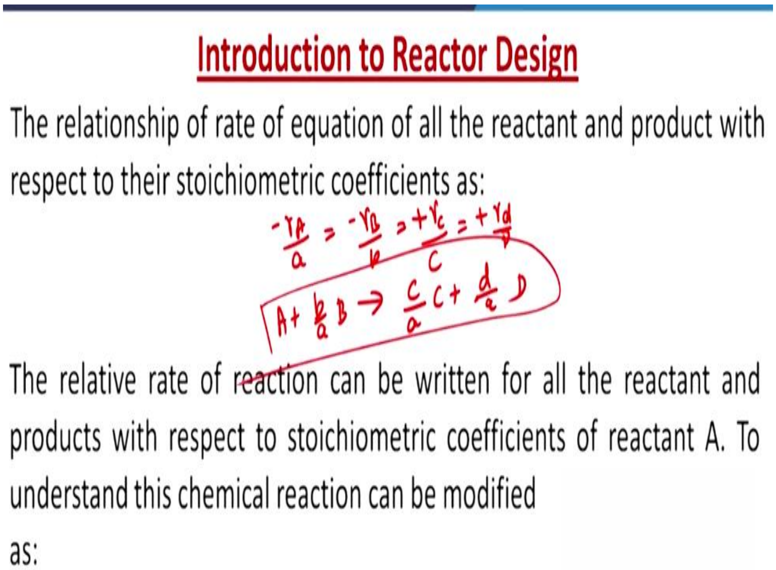

So, for this particular approach we may write this rate equation like this plus because c and d both are forming or sometimes r and s you may write like this if you try to correlate the things with the previous one. So, the modified chemical equation may become like this. So, this is your modified chemical equation. Now the relative rate of reaction this can be written for all the reactants and the products with respect to the stoichiometric coefficient of reactant A.

$$\frac{-r_A}{a} = \frac{-r_B}{b} = \frac{-r_C}{c} = \frac{-r_d}{d}$$

$$-r_A = -\frac{a}{b} r_B = \frac{a}{c} r_C = \frac{a}{d} r_D$$

Now to understand this the chemical reaction this can be modified further with attributed to this particular reaction. So, this is the modified chemical reaction or the chemical reaction.

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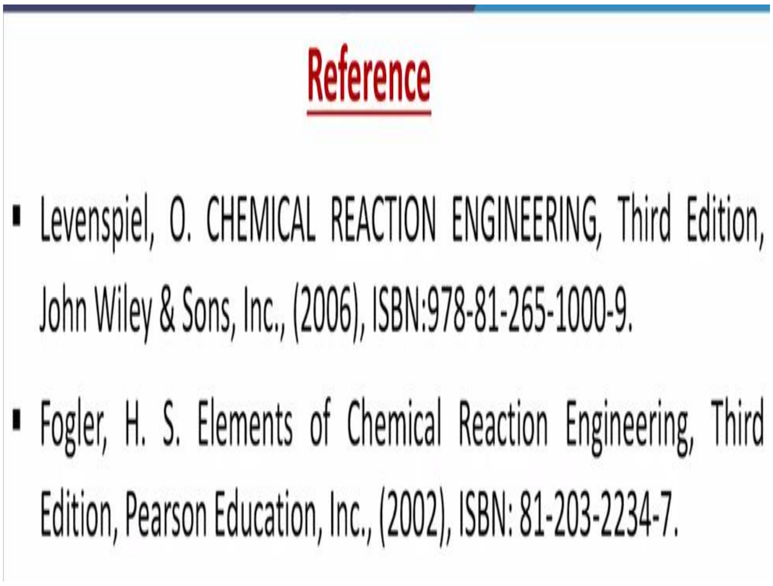

So, in this particular chapter or in this particular lecture, we have discussed about the different parameters associated with the reactor design. We have discussed about the mathematical equations, generation of mathematical equation. We discussed about the importance of a rate of a reaction and in the subsequent lecture we will discuss this concept of reactor design in detail. Thank you very much.