Advanced Chemical Reaction Engineering
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Lecture - 03
Design Equations-1

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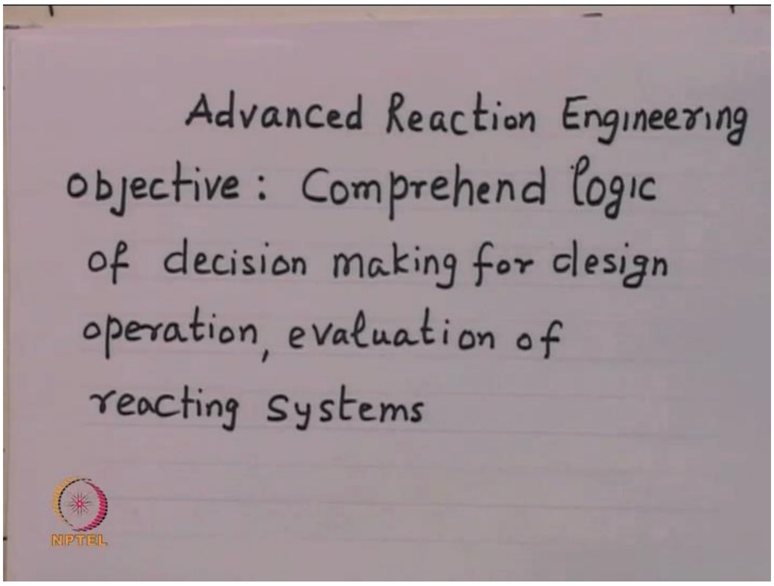

We are looking at advanced reaction engineering; the objective here is to comprehend logic of decision making for design, operation evaluation of reacting systems. So, it is a large subject in which we look at reactions has a central way of understanding what is happening? Let us look at some examples, where we might find this subject of much value.

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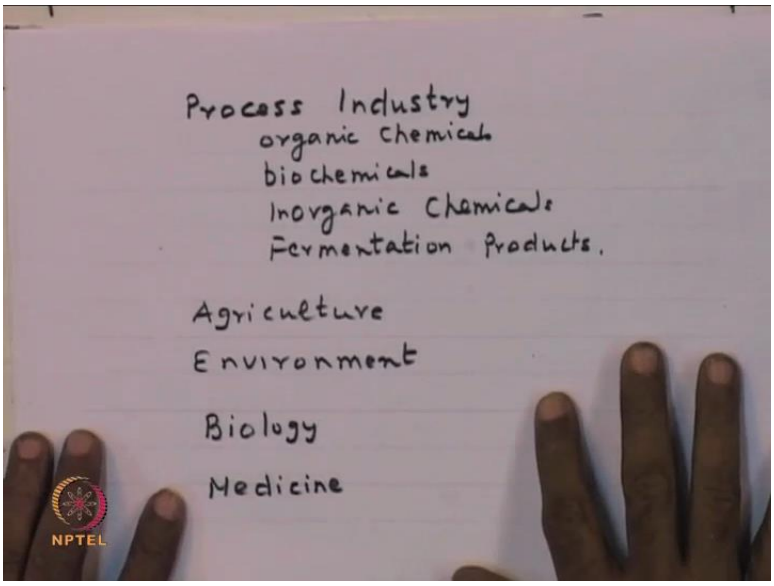

Process industry, for example, we make organic chemicals we make biochemical various kinds inorganic chemicals, fermentation products and then these are industries were they start with certain raw material to produce certain products. Our raw materials could come from agriculture; it comes from forestry; it come from mining; it could come from oceans in the form of various ocean products, all of which we used to produce various chemicals. Now, we could also be another way by which we look at reaction engineering is we want to understand agriculture in a larger way.

We want to understand what is happening in your environment or maybe we are trying to look at how medicine is performing on a certain organism may be human may be animal. Similarly, how certain medicine can interact with environment and so on. So, these are all situations where reactions are so central to what is happening in the system. So, to say that reaction engineering gives you some fundamental principle to be able to deal with small systems or large systems. What is our methodology?

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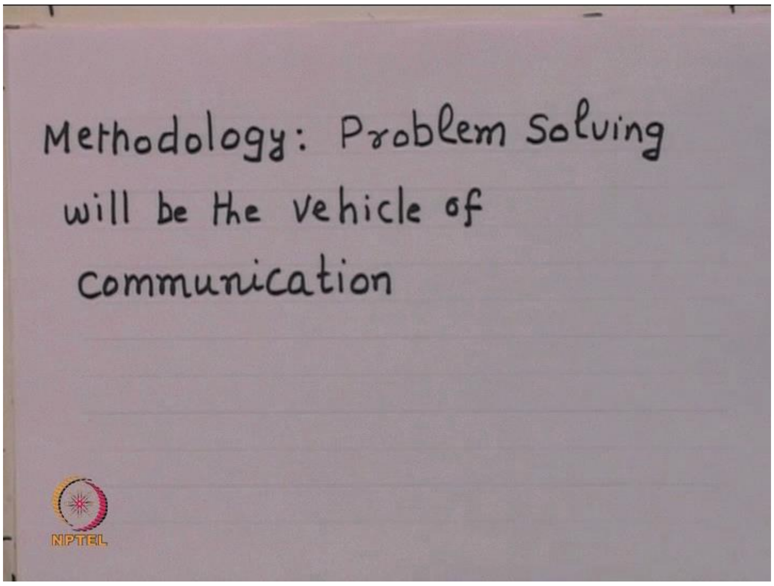

Our methodology in this course would be by enlarge problem solving; that means, we try to convey principles to you through solving small but carefully selected problems so that whether it is a process industry problem are from agriculture or environment or biology or medicine. Each of these situations, we will be able to comprehend by looking at these small but carefully selected problems.

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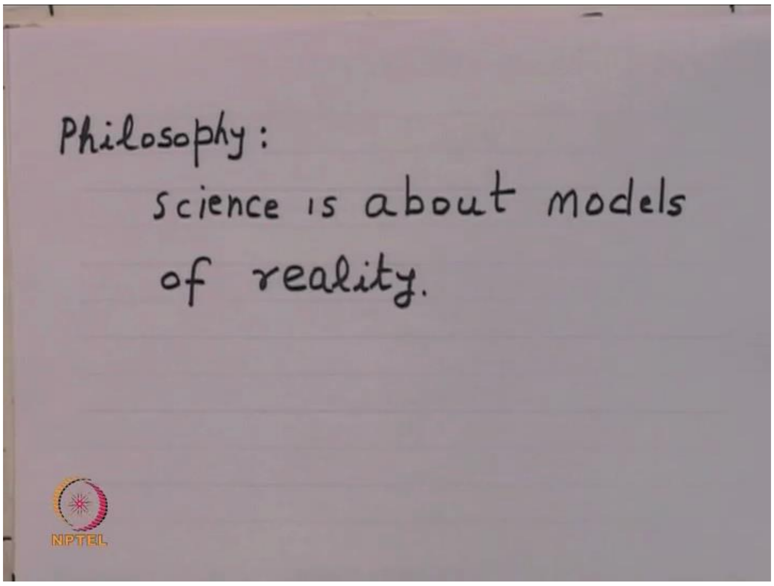

I mean, we have as you go along this course we will be formulating various models. Models, as we would always remember models have to be seen carefully so, we always remember that whatever we do sciences are only about models of reality. We like to understand reality we will models and we see how these models describe reality and if you describes well we except and as we understand more and more; we find these models are not so useful; so better and better models are required. So, the base point is the science are only about models of reality and to extent the model to describe reality we will use them when they not describe reality well we look for better models. So, this is philosophy with which we will look at this course. Chemical industry has been around for last more two hundred years now may be much longer.

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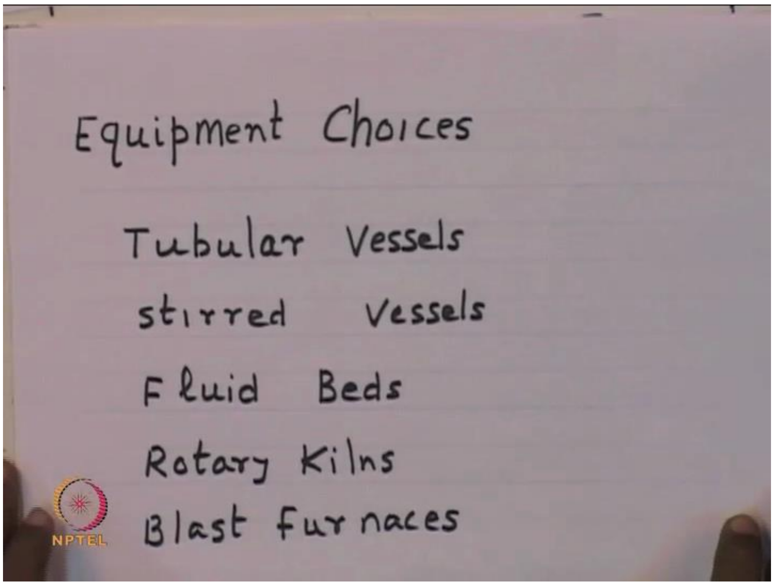

So, kinds of equipment that we will see in the chemical industry is tubular vessels, tubular reactors that is common in the petroleum industry; stirred vessels are very common in chemical industry; when we have fluid beds that you see in cracking industry; rotary kilns are very common in lime industry and of course, steel making and known for very long time blast furnaces or such equipment. On other words what we try to do in this course is to see how we can use or understand of the chemical reactions to build and design equipment and see how they operate. How they can be operated better? How best we can optimize its operations so that we produce our products safely, productively, economically so that we deliver useful value to society. So, whether it is tubular vessels, stirred vessels, fluid beds, rotary kilns or blast furnaces each of these choices are based on understanding of the reactions that we are trying to conduct.

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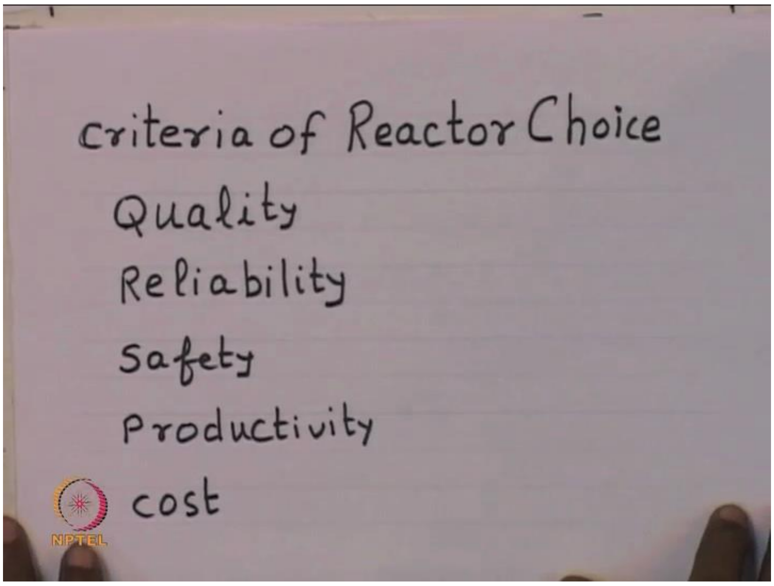

Now, the criteria that we will use the criteria of choice of these reaction equipment of course, depends upon on the quality of the product that we want to produce; the reliability with which you on make this equipment work; the safety feature there are associated with it; the productivity we desire and the cost that we would like. On other words, our choice will be dependent on the importance that we attach on to these five qualities. Of course, we say I mean this not that be compromising these qualities the fact is that all of them are equally important. Therefore, the criteria should be such that every one of the qualities is criteria are satisfied to the extent that is required for the process.

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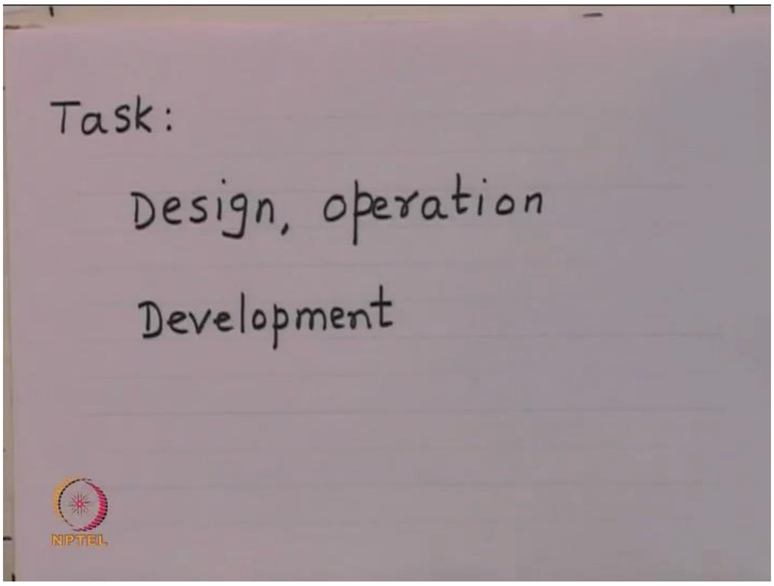

The task in front of us can be design; the task can be operation; the task can be development of a reactor design for a new application. Our principles must apply to all of these at all times so we need to develop principles and methods; so that we are able to address any of these situations that we would like to handle. So, to put this in the perspective this course advanced reaction engineering.

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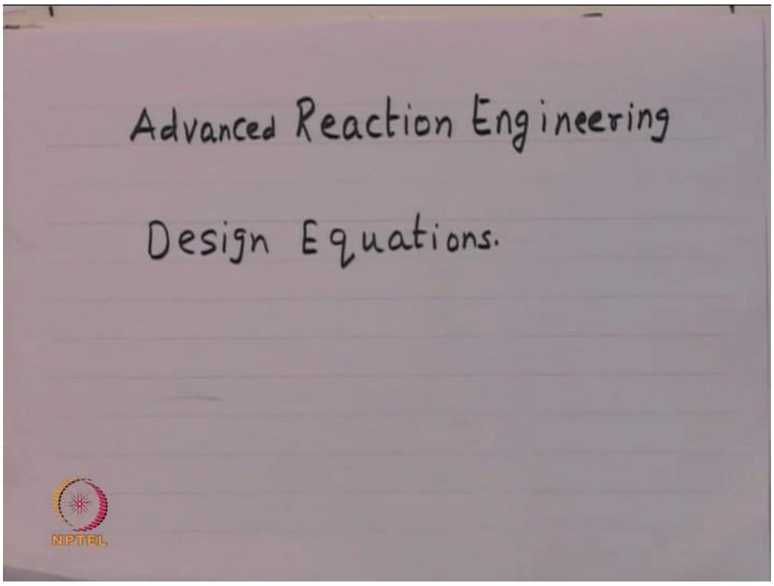

Essentially, we want to look at the design equations that are required to understand the equipment that we are going to design, to operate the equipment to performance function that we are looking for. So, let us get on with this task of reaction engineering design equations.

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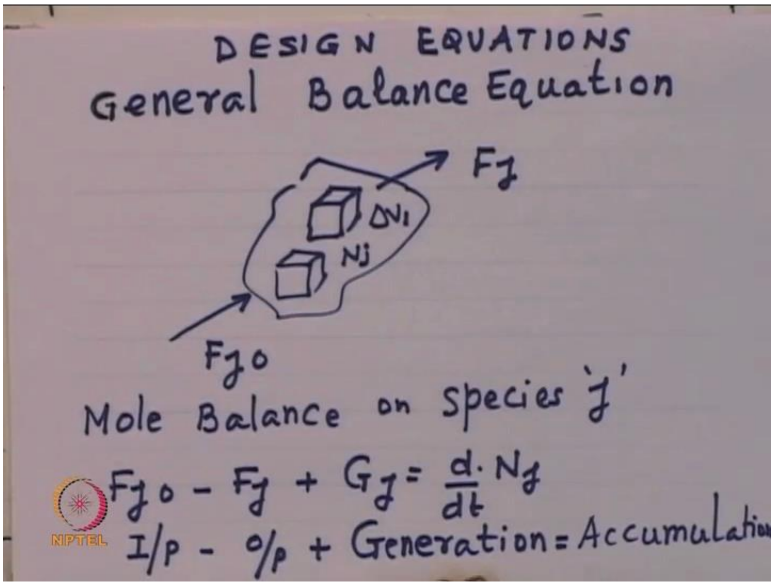

Now, this is a conceptual representation of what might be reaction equipment. Please do not think like this is how the reaction equipment looks like that is not the idea. So, we have an enclosure of an arbitrary shape deliberately chosen, in which a certain fluid F j at 0 is entry and it is leaving here; fluid enters and fluid leaves in the equipment. Now we can write a material balance; we call it is as a mole balance any other components that enter the system. F j 0 is the moles per time that entering the system and F j is the moles per time that leave the system, while G j is the moles per unit time which is produces in the system produce by means we can we consume it as a negative value. This difference would be the rated which the material is accumulated in the system.

On other words, input minus of output plus generation equal to accumulation is a fundamental statement of material balance; whatever comes in; whatever goes out whatever get generated; this combination that has to accumulate. Generation can be positive in which case this function is positive; it can be negative if it is consumed it is a negative value through general statement of material balance. Now, we recognize that this function G j this function G j; that means, they related which components is reduced or consumed by the point in the equipment this could to vary in the point to point variations. On other words, the rate of generation of this component can be different points in the equipment you must take into an account.

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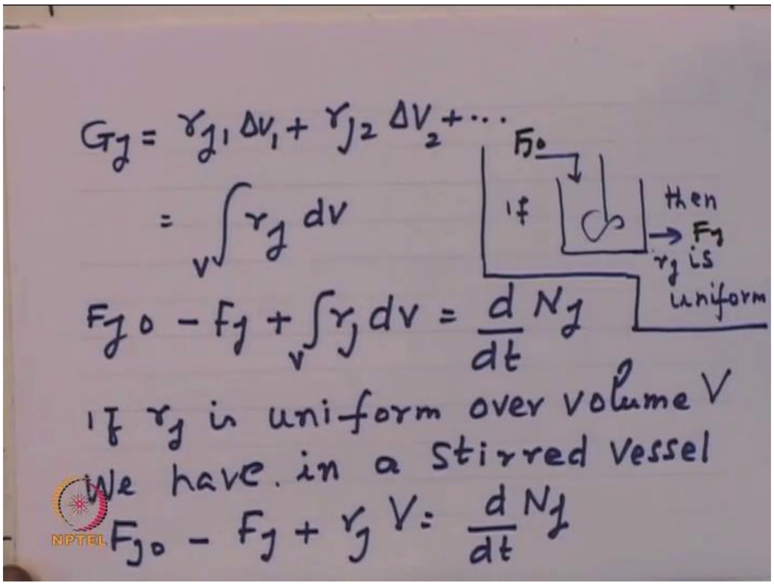

So, keep in that in mind what you are said in that at different points one two three four five upto n r j 1 is the rate of generation component j delta v 1 is the volume of the elemental volume. Similarly, r j 2 is the rate of generation elementary volume delta v 2 upto n. On other words rated which the component j is generated is an integral of r j multiplied by dv. So, r j dv is the rate of generation of component j. So, if you substitute this into our general statement here material balance replaces this G j by r j times dv. So, that we have more general statement of the composition equation F j 0 minus of F j integral r j dv equal to d by dt of N j. Now, it could so happen that the equipment that we are dealing with is an equipment where there are is a stirrer so that the composition temperature in other intensive variables are essentially the same and different points in the in which case called stirred vessel.

So, if you have stirred vessel into its continuous input of component the continuous output of component j then, we have we are continuous input of component j continuous output the stirred vessel in which case we can say that r j is uniform at every point inside the equipment so that we can take r j outside the integral therefore, this equation can be written as F j 0 minus of F j plus r j times v integral dv is v equal to d by dt N j. Other words out statement of material balance for the case of stirred vessel can be written as F j 0 minus of F j plus r j times v equal to d by dt N j. Let us look at this some more detail.

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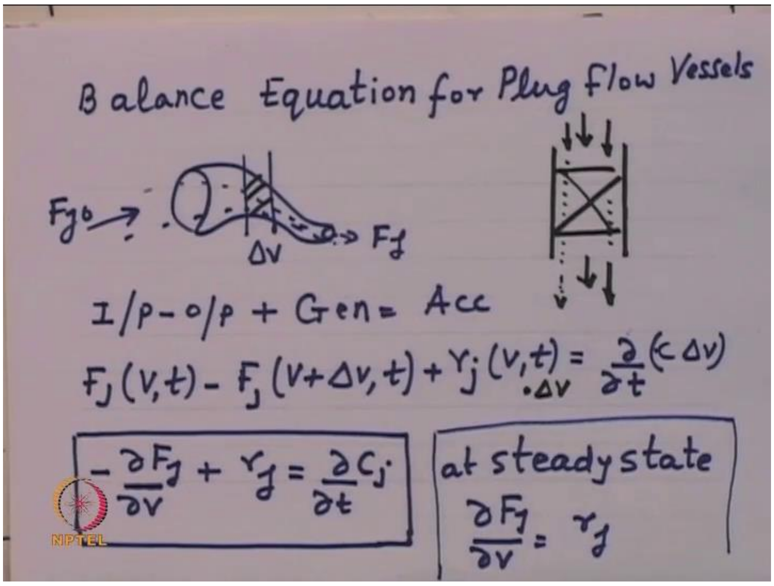

Suppose in state of stirred vessel instead of stirred vessel, we have a different type of vessel which is often seen in the process industry which is called as a tubular reactor. What is the tubular reactor? We have a pipe of a chosen diameter, perhaps we have a catalyst inside and fluids come this way; let us say and this is out way a tubular reactor. Now, this is trying to represent a general situation where you have a vessel of an arbitrary shape through which component j is entering component j is leaving; component j is entering and leaving F j 0 is entering F j is leaving. We want to write a material balance on an elemental volume delta v so, this is the elemental volume delta v are which you want write a material balance.

So, we notice here that F j at v at any time t F j at v plus delta v at any time t plus r j times v at any time t equal to this is the total amount of multiply with delta v. So, this is the statement of material balance for a flow through what we call as plug flow vessel. By plug flow what you mean is that every fluid element is that enters here moves through the equipment without recognizing the existence of other fluid elements. On other words as the fluid moves through the equipment it does not mix with other fluid elements. For example, what is mean said here suppose the fluid element comes here it moves through and gets out; another fluid element that enters here it moves through and gets out. On other words this fluid element moves through and this fluid through this and they do not recognize existence of each other.

As a result this is called as the plug flow there is no inter mixing between these two fluids and such situations when we write material balance in the element F j at v F j at v plus delta v rate of generation with the component j this is the difference that accumulates. So, if you take the as delta v tends to 0 and so on. This how the material balance looks like under the unsteady state; when it is steady state where this term disappears the question which like this. On other words what we are trying to say here is there are two types of equipments; ideal equipment that you will see in the process industry.

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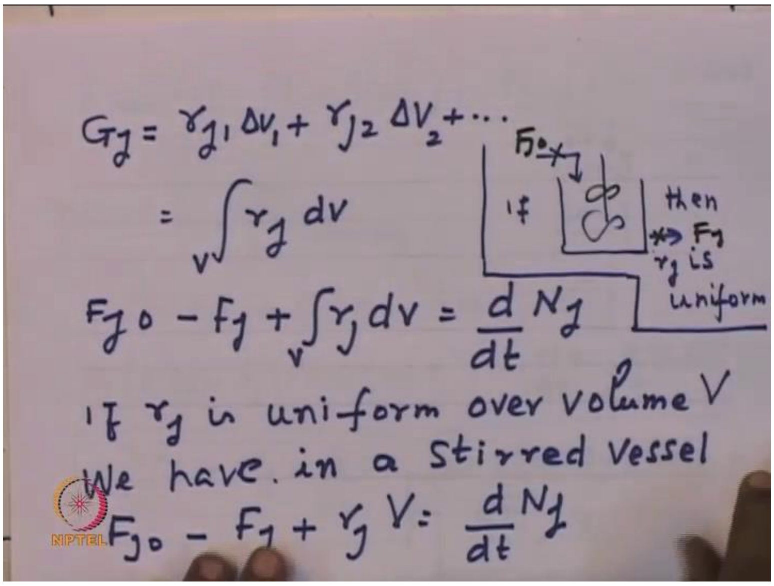

Equipment number one, we may pointed out is a stirred vessel. This stirred vessel could be operated such that it could be a batch in the sense there is no continuous input and continuous output, it is still a stirred vessel there is a stirrer; there is a composition is maintained.

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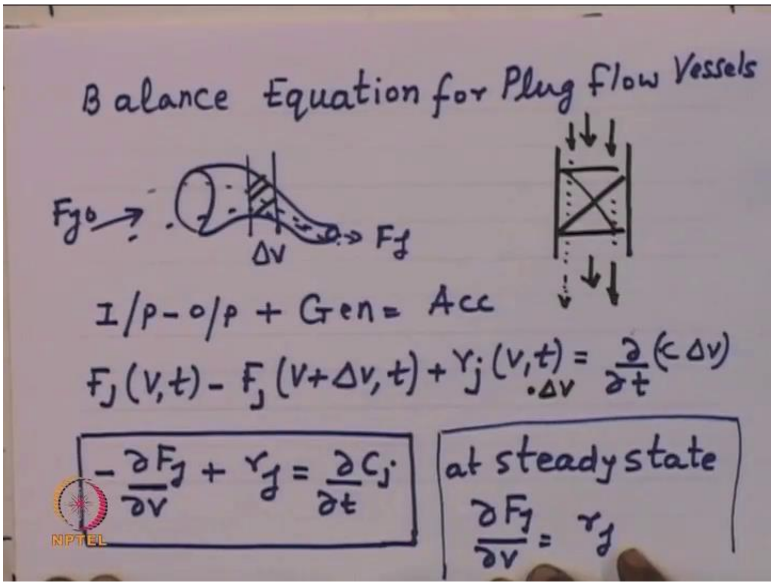

The other kind of equipment is what we have here is tubular equipment where materials move through and then exit without mixing with each other that is called as plug flow vessel. The equations that describe if the variation of various properties for a stirred vessel is given by this and for plug flow vessel given by this. For a plug flow vessel at a steady state del by del v of F j is given by rate of generation of j and for stirred vessel equation is already shown. Now, these two types of equipment what we call as plug flow this is for a case of plug flow equipment.

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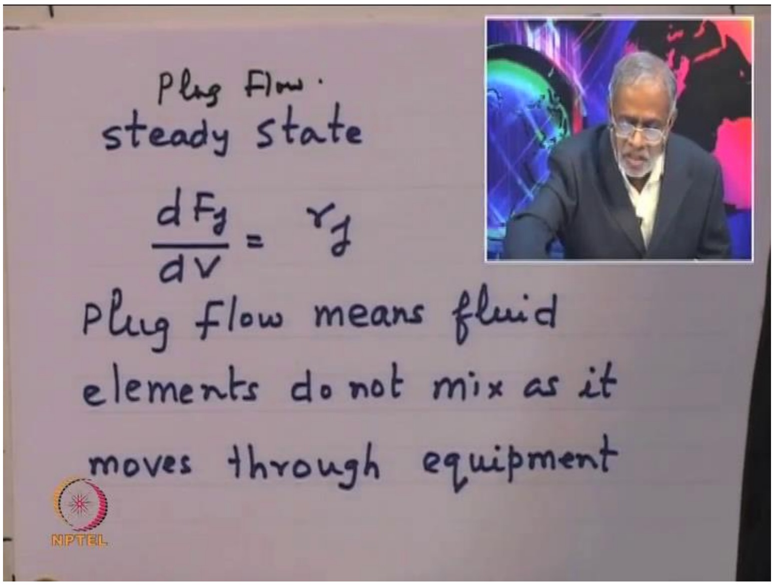

So, you find that plug flow equipment are very common particularly, in the process industry dealing with catalyst. Because this pipe holds the catalyst and the fluids can enter and leave; therefore, the catalyst that is performing work for you can be changed assignment activity goes down. That is the kind of equipment most popularly used in the process industry we will deal with fluids and mode of heat etcetera. Particularly, in smallest scales, you will find stirred vessels in batch and continuous mode. On other words what am trying get across to you is that you have the stirred vessels, which are commonly used for smaller scales operations. Where do you have either in batch operations or continuous operations?

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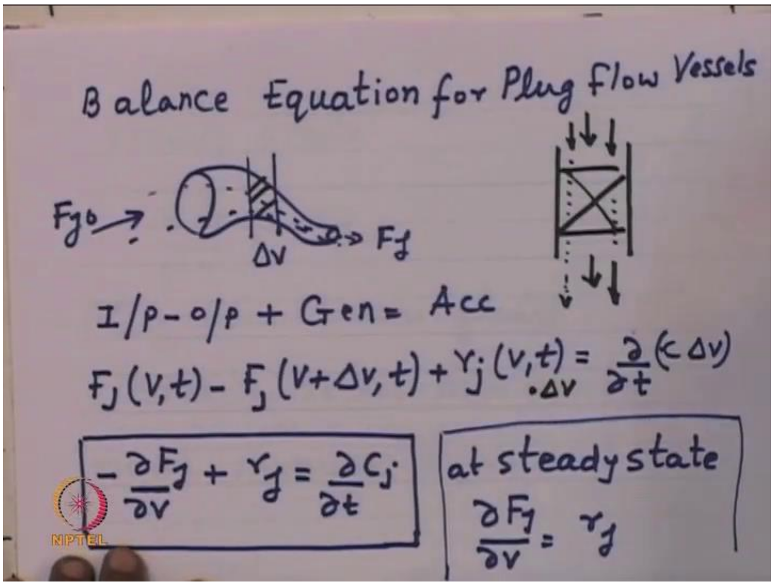

You have this plug flow vessels particular for catalytic reactions; mostly in very large scales they have a catalyst, which is continuously used for processing a certain material that selecting a final product. So, batch vessels continuous stirred vessels as well as plug flow vessels are the most common thing that you will see in the process industry. We have set up equations both for batch and stirred vessels here and then we are set up equations for steady state and unsteady state for the plug flow vessels. Our job now is to see how reactions perform in these ideal vessels. How do reactions perform and what we can learn from the performance of the reactions?

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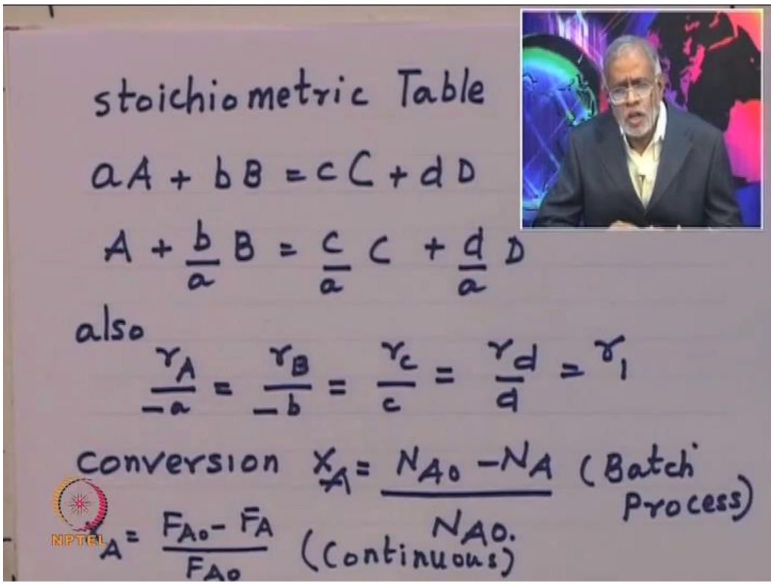

Let use just to illustrate let us just assume that the reaction of this form a A plus b B giving you c C plus d D takes place in our reaction equipment. Now if you choose a as our reference species then we can divide throughout by a so that our reaction now looks like A plus b by a B plus c by a C plus d by a D. This is assuming that this is component A is our reference. Now, we know that the reaction takes place at certain rate if I call that rate of chemical reaction as r A; if I say that rate of reaction of component A r A understanding a basic chemistry that r A divided by minus of a equal to r B divided by minus of b equal to r C divided by plus c equal to r D divided by plus d.

On other words this ratio rate of reaction A divided by tachometric coefficient with appropriate sign for a given reaction there are equal and therefore, I turned this r 1 sometimes called as intensive rate of reaction. Now, how do we understand conversion? We understand conversion at steady state conversions are typically we start with so many moles away and end of the reaction so many moles unreacted. So, we express the amount of component A converted with respect to what is started with that is gives to the conversion. In other words, the whole meaning of conversion requires you to recognize certain starting material or reference. So, our reference for defining conversion is N A 0.

If you have a batch process you have a continuous process this N A 0 is moles if the continuous process X A is defined as with respect to the reference F A 0, where F A 0 has the units of moles per time. So, whether it is batch or continuous we defined conversion with respect to certain reference. For continuous process, we have taken F A 0 reference species and for batch process we have taken N A 0 as a reference. Choice of reference is always your choice in the sense you can prefer defined with respect to your reference. Generally, a reference component giving limiting substrate or limiting agent that is in the reaction that is how it is normally reference is ok.

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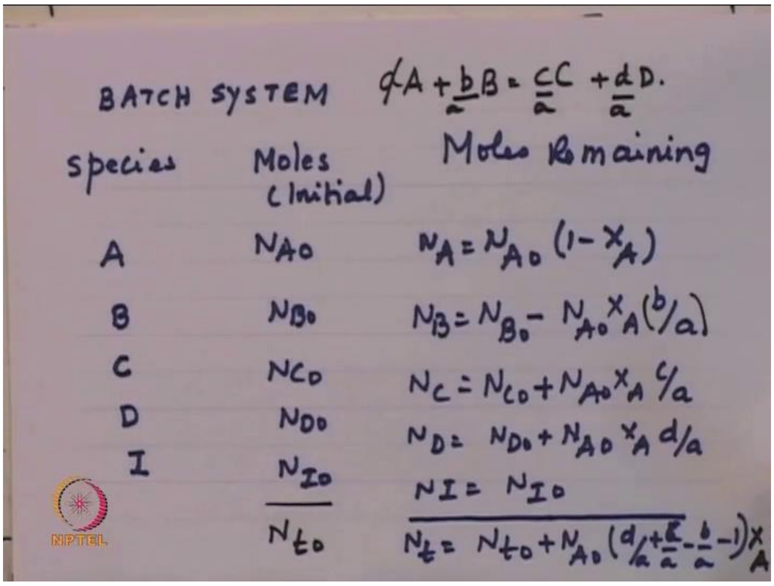

Let us say we have a batch system where the reaction a A plus b B just we write it down on the scale our reaction is a A plus b B equal to c C plus d D all of you divided throughout by a it will like this . So, for this reaction if you look at species A B C D and I; I is inert typically every system comes into inert. So, you starts with so many moles N A 0 N B 0 N C 0 N D 0 N I 0 and so on. Therefore, as per stoichiometry what we have written is if X is a extensive reaction or conversion. So, the unreacted a is given by N A equal to N A times one minus of X A, whose definition and similarly N B is N B 0 minus of N A 0 X A multiplied by b by a.

So, this term b by a this term comes because of the stoichiometry as we are represented there. So, as per the way we are define conversion and the way we are taken the chemical reaction; we can write what is the unreacted amounts of A B C D and I in the system at any given conversion. This follows directly form stoichiometry you can add up all this. When you add up all these you will find it is number of moles we start with is N t 0.

When you add up all these moles this is so many moles to have coming in and so many moles are going out.

When you add up all these you notice here this is N t N t 0 and all these terms common N A 0 X is common and X A; this term inside d by a plus c by a minus b by a minus 1; this term the effect or the chemical reaction. So, what we get here from stoichiometry number of moles we start with the number of moles we get; then this is the certain amount of reaction X A.

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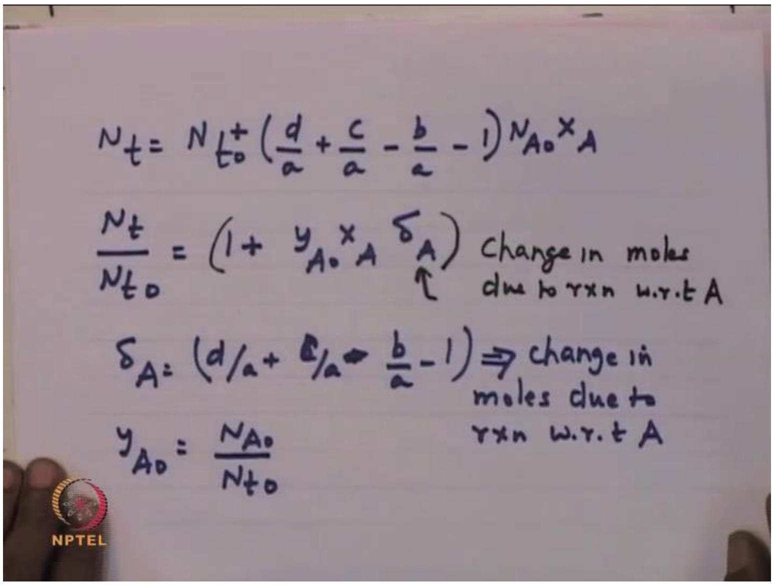

Now, we can write number of moles at the end of certain extensive reaction certain conversion X A is given by N t 0 plus this term the effect of the chemical reaction as expressed with respect to component A, which is what is called as delta A. Delta A is meaning of delta A is change in moles change in moles due to reaction with respect to the reference component A. On other words delta A tells you what is the number of moles change that comes because of the reaction d by a plus c by a minus b by a minus 1; this is the known quantity for every reaction. So, what we get from stoichiometry is that given a conversion X A given conversion X A N t by N t 0 is given by this relationship.

y A 0 is the mole fraction of component A by the start with the N t 0 is the total number of moles, which we start and delta A is change in moles due to reaction expressed with respect to component A. So, in other words this representation tells us what is the number of moles at any conversion at which the reactor working. Now, what is important is what we have done here what we have done here with respect to component A; we can do with any other component does not matter. So, just put it in the perspective but I have said here is that.

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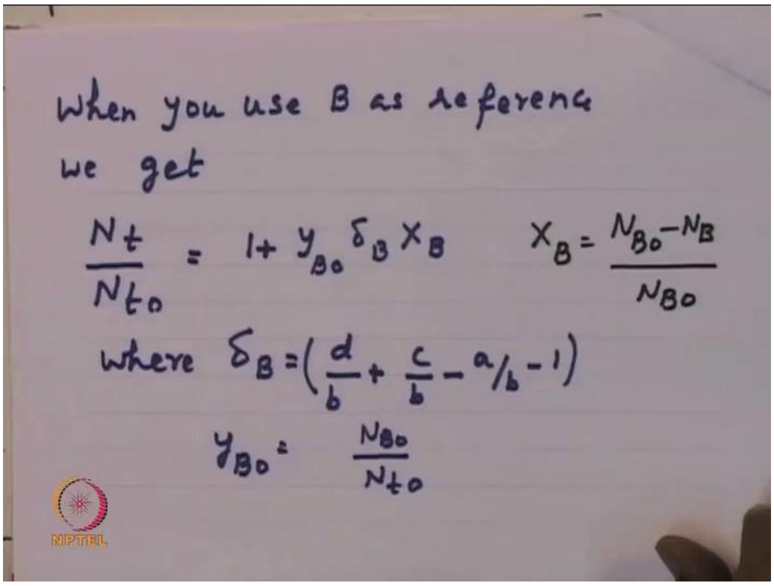

If you chose B as a reference species then your equation look like this instead of y A 0 instead of y A 0 here y B 0 instead of X A; you will get X B and what is the X B what is the X B; X B is generic X B equal to N B 0 minus of N B divided by N B 0. On other words, X B is the conversion as measured with respect to the component B. We recognize that inner reaction this could be different in measure conversion with respect to component A and component B there could be different.

Now if instead of for batch systems so we talked about the stoichiometry all the stoichiometry we have talked about is considering our system is batch system. By batch what we mean is we have equipment, which is a vessel which is got no outlet and no inlet; certain amount of fluid is inside the equipment and then these are the changes that we are going to observe.

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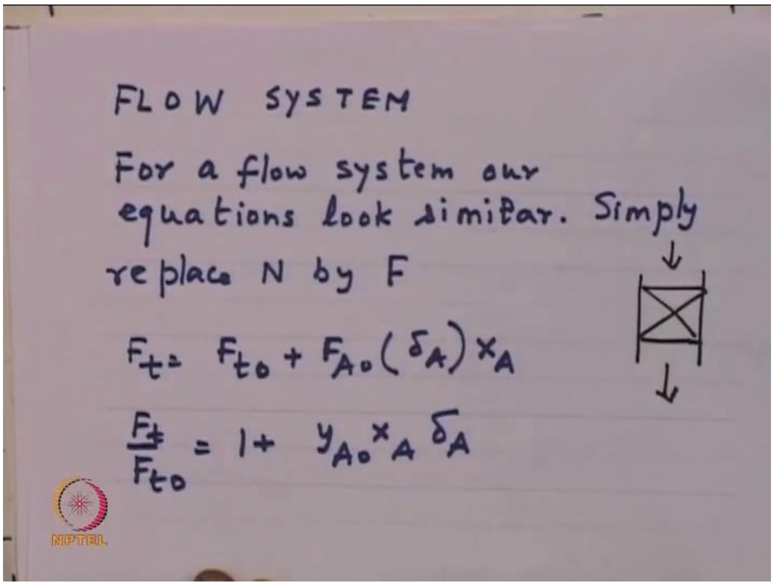

But we could also have a system where there is a continuous input there is a continuous input and continuous output like a tubular reactor; there is a continuous input there is a continuous output. So, how do we deal with systems where there is a continuous input and continuous output? So, when we have a flow system our equations now look exactly the same that is not difference or stoichiometric still does not change. I notice here this here is to writing if N A 0; I could written in F A 0 F B 0 F C 0 F D 0 F I 0 F t 0. On the other words as per the stoichiometric concern it does not matter whether you are talking about plug flow system or a batch system. Therefore, whatever relationship that we get for n t is the same we will get when it is for f t because stoichiometric does not get affected because of flow etcetera.

So, we can say now F t the total number of moles giving the system is F t 0, which is total number of moles entering the system multiplied by F A 0 X A multiplied by delta A. Same like here N t equal to N t 0 N A 0 this is delta X A. So, essentially what we are saying that if the flow systems then total moles leaving is related to the system with same kind of equation that we have done for the batch system. So, that F t divided by F t 0 is given by 1 plus y A 0 X A delta A; previously we have N t divided by N t 0 given by this. So, whether it is a N t by N t 0 or F t by F t 0 the right hand side does not change because these are coming from stoichiometric. Now have we set all these things let us go a little bit forward and see how we look at various kinds of design equations for our systems?

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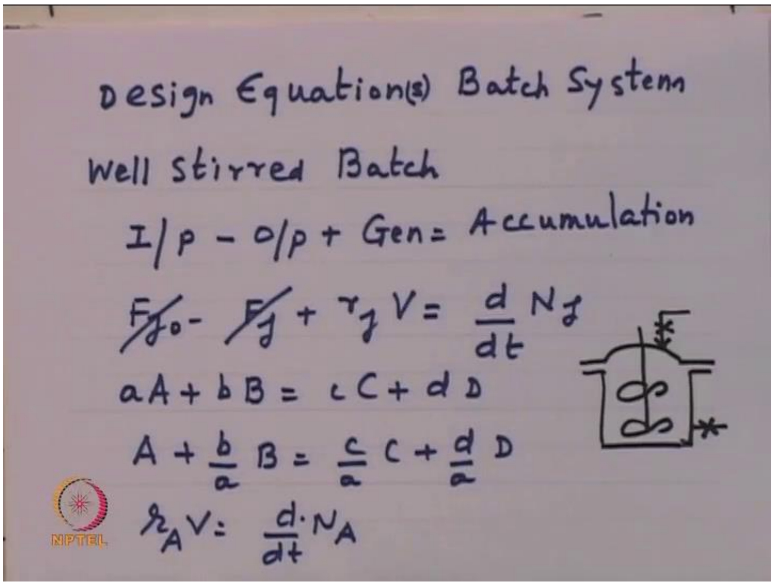

First system we are taking that is batch systems. Let me just remind you what the batch system is or batch system looks like this. You have a vessel the vessel is closed it is well stirred, which means the composition are same at different points there is an inlet, but this this is closed; there is an outlet which is closed. The idea of this inlet valve and outlet valve so that we can charge and discharge. So, as for the reaction is concerned during the reaction there is no inlet and there is no outlet, whatever is taking inside the equipment that is what brings about the reaction? So, the case of the batch system where there is no input where there is no output there is only generation and accumulation. Therefore, first term and second term disappears therefore, you have r j times V rate of generation of the component equal to d by dt of N j.

So, this is the statement of the material balance for a batch system that rated which the reaction takes place equal to the rate of accumulation in the system. Now our reaction is given by a A plus b B equal to c C plus d D or in terms of component reference it is looking like A plus b by a B equal to c by a C plus d by a D. Therefore, now we can say if A is a reference species r A times V just replacing j by a we have r A times V equal to d by d t of N A. So, statement of material balance for a batch system is simply r A times V d by dt of N A. Now we can go forward, we will taking about stoichiometric table.

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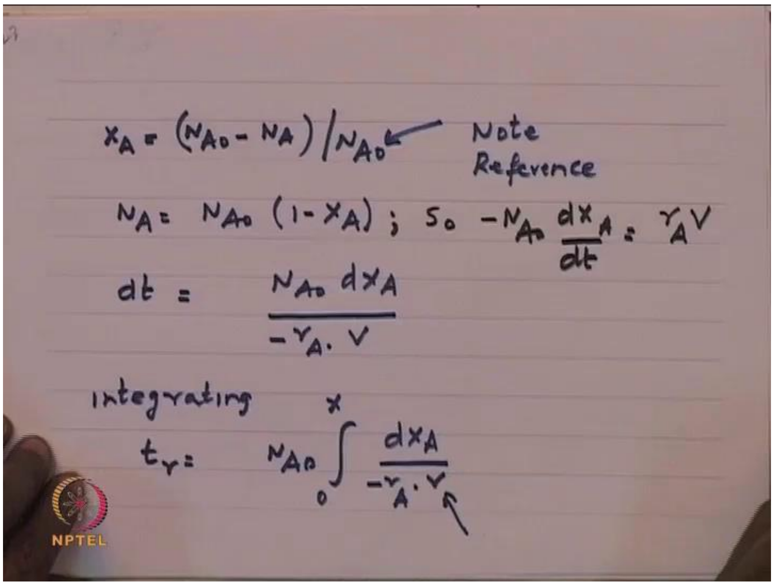

Now, something that we know that conversion is defined as N A 0 minus of N A divided by N A 0. A point to be noted here is that N A 0 is a reference; this reference is our choice. This particular case we have taken A as the reference. Now as a result of the this representation know this N A is given by N A 0 times 1 minus of X A. On other words if we look at batch reactor we find minus of N A 0 dx A by dt equal to r A times V; this is the statement of the material balance. So, that we can see dt equal to N A 0 dx A divided by minus of r A times V, when you integrated this if the reaction time is N A 0 dx A divided by minus of r A times V.

Notice here that volume volume volume effect appears here. On other words if volume of the reactor changes during the process of the reaction, where the effect should have to be accompanied here. If the volume is constant you can take out of the integral so that it becomes N A 0; so that t r N A 0 times dx A divided by minus of r A times V familiar representation takes place it is so, why does this is constant important issue we must bear in mind.

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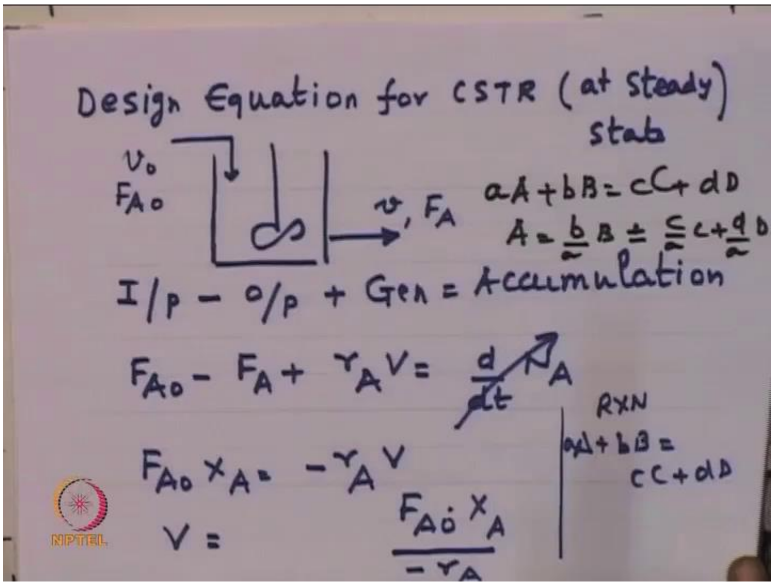

Now, lets us take another very common instant that you might see in the process industry what is called as continuous stirred tank reactor. Now, stirred tanks are examples were the fluid comes in continuously; fluid leaves continuously. Batch equipment please recalls batch equipment we said the process works the process works and during the process there is no input. We set this batch equipment is an instance where there is no addition or removal of material as the reaction takes place. That is the batch equipment, which are all the raw materials close all the valves conduct the reaction at the end of the reaction time; you open this valve to discharge the product.

Now, a continuous reactor is of continuous input of fluid continuous removal of fluid, a reaction takes place inside this equipment continuously. Therefore, we are able to continuously withdraw the product at the rate that we are desire. So, continuous reaction what is called continuous stirred tank reactor; one example of process equipment by the you will produce the product continuously. On other words, you do not have to worry about charging time discharging time and so on, which could be very significant in the batch process. So, all the charging and discharging of material is eliminated only on the process time is what is of concerned to you and this way you are able to produce large quantities of materials.

But an advantage of the continuous process is that we do not use time during charging and discharging. Now, let us see how the equation looks like. Our statement of material balance does not change input minus of output plus generation equal to accumulation these are fundamental statement of conservation of mass. Our input is what if are reaction once again let us recognize let me write down once again a A plus b B equal to c C plus d D and A as reference it becomes b by a B plus equal to c by a C plus d. So, we are still considering same reaction with A as the reference. So, we have input input is a F A 0 we can see here input is F A 0 output is F A; you can see here rate of generation of component is A and d by dt of N A and their operating at steady state.

We will look at unsteady state of situation later on for the moment let us assume let this process is running at steady state. What is meant by steady state? By steady state we mean if you look at composition of the system at any time you look at composition of the output at any time. We will find composition inside the equipment and composition exit at the same; that means, it does not change with time. Steady state is an instance of a process operation, where the composition that you measure the exit does not change with time. Composition that you measure inside the equipment with time does not change its time; that means, it is steady with respect to time under situation where this is steady if the equation F A 0 minus of F A plus r A V equal to d by dt of N A.

On the right hand side which represents accumulation because it is steady there is no change with respect to time therefore, d by dt of this will go to 0. Therefore, the right hand side is 0. So, steady state representation of material balance gives you F A 0 times X A equal to minus r A V; because right hand side is 0. Please recognize F A 0 minus of F A equal to r A V comes from the fundamental definition of X A. We define X A as F A 0 minus of F A divided by F A 0; that is how X is defined that is why we write this term in this form. So, that this representation gives us volume of continuous stirred tank reactor is given by F A 0 times X A divided by minus of r A.

So, a continuous reaction in which you have CSTR bring about this reaction volume of the equipment is given by F A 0 times X A divided by minus of r A; F A 0 is something you know X A you can measure and r A is the chemical kinetics at which the reaction occurring. So, right hand side known quantity therefore, given the chemical kinetics given the extent to which you must react given the production that you want all these can be taken together to determine what is the size of the equipment which must design for.

Now, why is it that moved away from batch equipment continuous equipment like CSTR there are many reasons for this batch to continuous is the decision that (( )) take depending upon the scale of production. Generally, you find continuous production of preferred if the scales are very large the scales are small of course, the batch productions are preferred. But that is not saying enough lets also recognize the when you have some products which are very expensive, where you require very careful control of the process during the process of reaction the general preference is to batch so that you can address all the issues that that is required to be addressed in the course of reaction.

So, there are certain advantages in doing batch processing and are there are advantages using continuous processing and the decision will be a decision that is taken based on technical economic and commercial issues.

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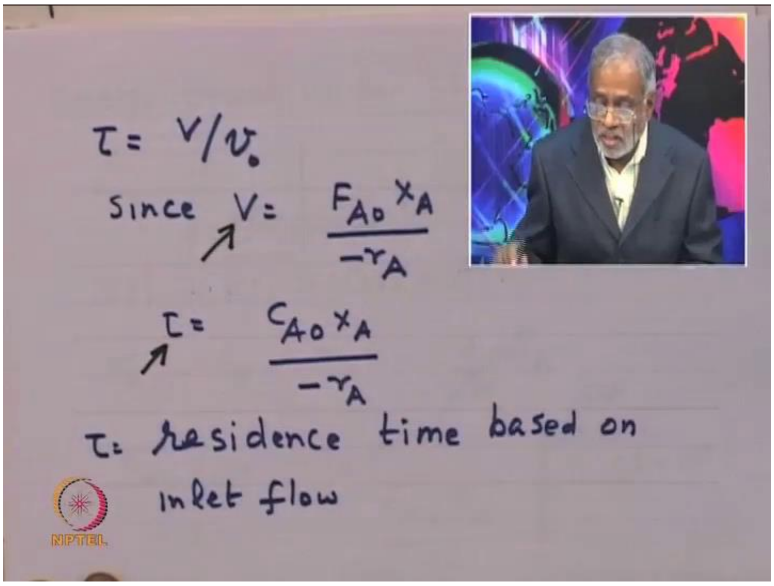

Now, what we are now saying is that if our stirred tank continuous CSTR design equation is this recognizing that residents time this actually volume of the equipment divided by the flow at the inlet. Then, we can write our design equation in terms of V; we can also write in times of resident time torque, which looks like this. On other words this is in terms of volume this is in terms of residents time they are stating the same thing the residents and reactor volume are related depending upon the volume flow at which we process the fluids.

So, this is the fundamental statement of design equations for CSTR or this may be another way of saying this is the equation for CSTR. If you know the chemical kinetics if you know the extent, which you want to react and if you know this fluids you can say what is the size of the equipment that is required for your process. What does happen in the process industry that there are situation where you may need there are no one stirred tank there are many stirred tank in sequence.

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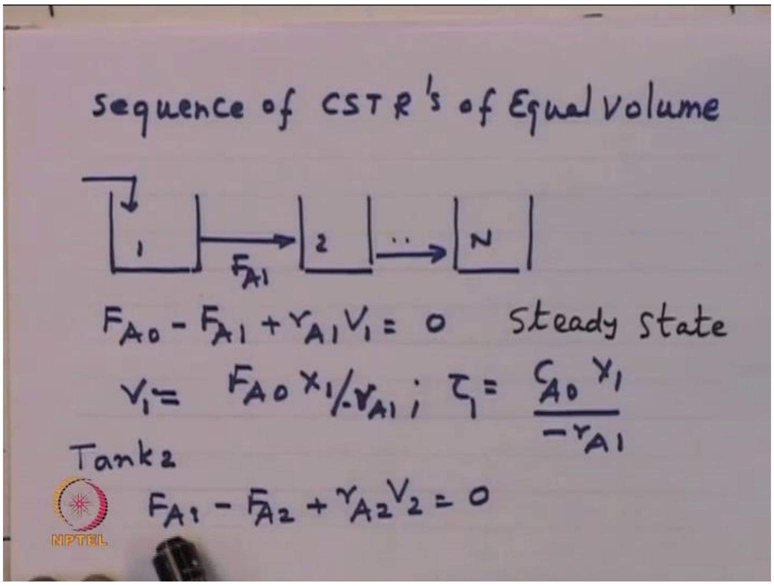

There are situations which require many times to be operated in series, but more importantly this sequence of stirred tanks gives us certain inside what happens in the process. Let us say look at what this sequence tells us this sequence tells us that if you look at tank one; input output generation equal to 0 at steady state; we have study all these are steady state; that means, we are writing a material balance at steady state. We will come to unsteady state at later date first now we are looking at steady state.

Therefore our statement of material balance leads us to size of the equipment given by F A 0 X 1 divided by minus of r A 1 or residents time given by C A 0 X 2 by minus of r A 1; that means, the residents time in tank one is given by this equation C A 0 X 1 by minus of r A 1. Now, if you write material balance for tank two which is F A 1 minus F A 2 input output generation is equal to 0, where this is the rated which the reaction occurs in tank two; r A 1 is the rated which the reaction occurs in tank one. therefore, this equation is the way of understanding what is the size of V 2 that is required.

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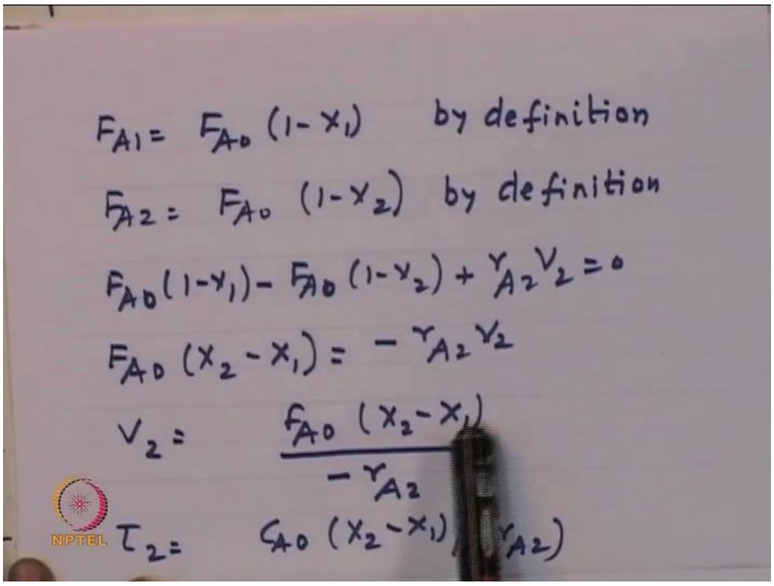

So, we can simplify this write our material balance; material balance this is our material balance for tank two. What is written once again in the next page F A 0 input output generation equal to 0. We find that the size of reactor two equipment two can be given as F A 0 times X 2 minus of X 1 X 2 is what is the X 2?

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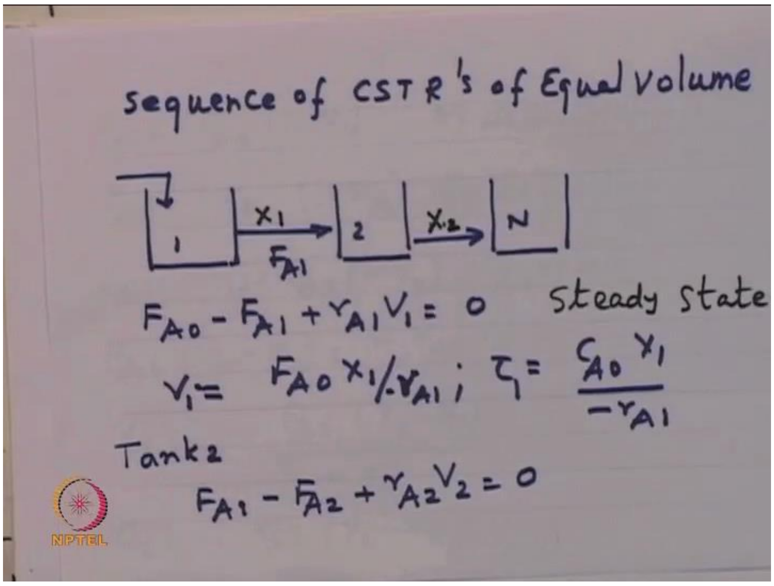

X 1 is conversion at the at the outlet tank here; X 2 is conversion here, what are we saying here?

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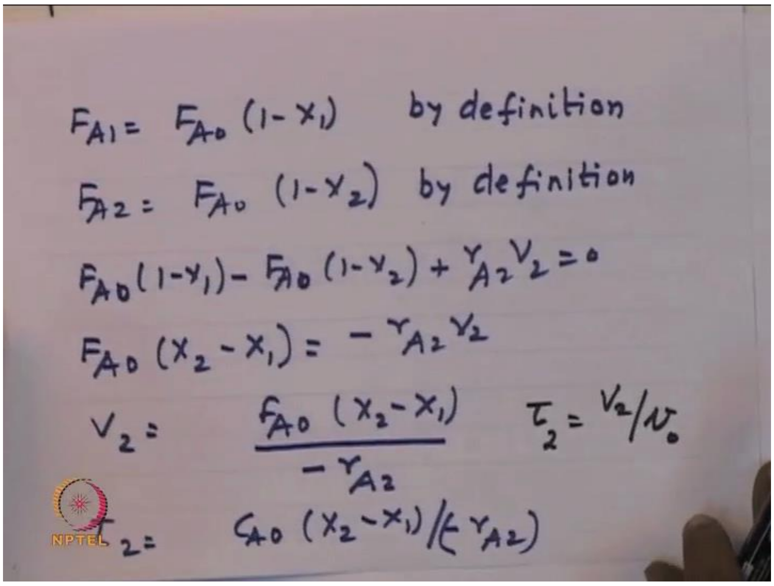

What we are saying here is that; the size of tank two depends upon F A 0 times X 2 minus of X 1, what is the X 2 minus of X 1 it is the moles of component A undergone chemical reaction in tank two. What is r A 2? r A 2 is rated which chemical reaction occurs in tank two. So, the total moles converted divided by the rate of conversion using size of the equipment. So, it is stating the obvious it is nothing new I have been said obvious being said but said in a form this is useful for calculations.

So, what do we get, the size of the equipment we told we want to express in terms of resident time our residents time is defined as equal to V 2 divided by v 0. So, we have size of the equipment two, I mean reactor two is given by C A 0 the conversion change divided by the rate of change of reaction. Now, we can continue this whole process and then say for tank three tank four tank five and so on.

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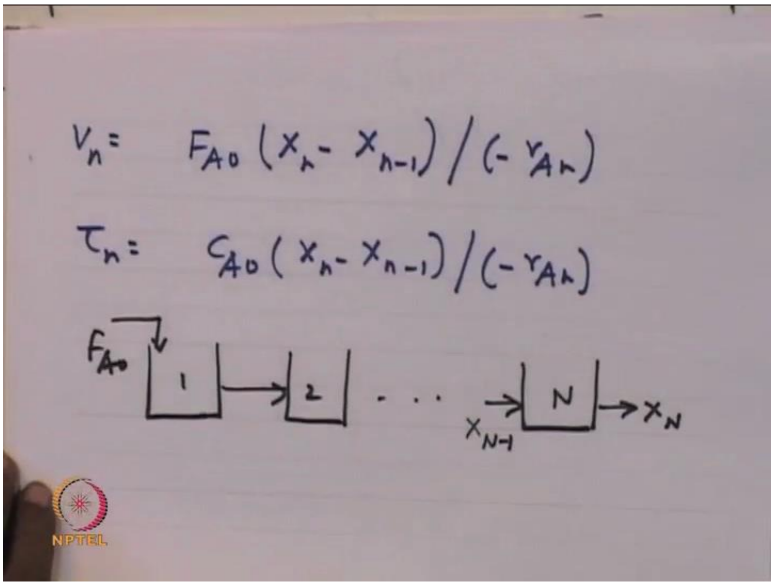

We can say for tank N we are looking at its F A 0 times X N minus X N minus 1 divided by minus r A n, where what is F A 0 F A 0 is recognized, we have N tanks here; tank one and tank two and then tank n. This is tank N, 1, 2. Now inputs this is the F A 0 this is what is coming out is X N. So, what we are saying is that size of the tank is V n this is n if F A 0 what comes here multiply by what happen this is X N minus of 1; what is coming here is X N minus of 1 you see so, X N n minus of 1. This is difference change in conversion this divided by rate of chemical reaction. So, it is stating is obvious, but in forms that is very useful to us for doing calculations. So, what are we said what we are said is that if you have if you have tanks in sequence instead of single tank tanks in sequence.

When we find that we can use a same statement of material balance to find out; what is the size of the equipment one tank one; what tis the resident time in tank one. Then we can see what the size of the equipment two is; what the resident time is in tank two. Similarly, we can say what the size of the equipment n two is; what tis the resident time in tank n. So, our statement of material balance helps us to calculate all this because it is put in that form. Suppose, as we said when we started this we said we have two types of equipment that you will see in the process industry. One that is what is called stirred vessel that is mechanically stirred; the other equipment you have plug flow vessel, where there is no mechanical stirring inside the equipment.

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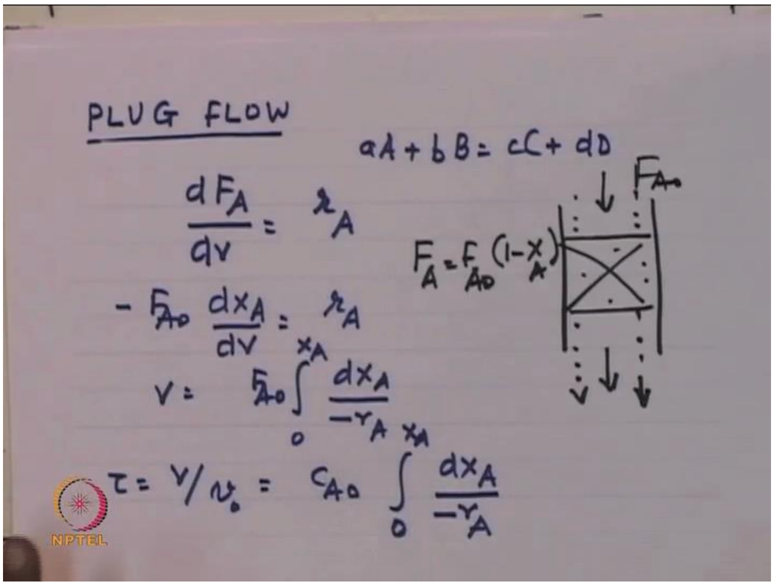

That means the plug flow equipment you have let us say a pipe may be inside the pipe there is a catalyst and the fluid is coming in and going out; there is no mechanical equipment inside here to do stirring. So as a result but expects but there is plug flow plug flow what we mean is that the inside without mixing with each other; so this is plug flow vessel equipment. Now, we are already derived what is our design equation for a plug flow equipment for a reaction like this. We already said this d by dv of F A is r A. What are we saying here what we are saying is that d F A by dv is what rate of change of moles of a per unit volume per unit time. So, rated which moles are changes per unit volume per unit time that must be equal to the rate of chemical reaction.

It is stating the obvious what is trying put across to you that every equation that is written here is that stating the obvious. It is in a form that we can understand from first principles nothing new being said. Now, we can represent this F A from our stoichiometry; what we are said in our stoichiometry we said in our stoichiometry F A is equal to F A 0 multiplied by of 1 minus of X A. This is how it is defined this conversion itself defined like this. Therefore, we are able to substitute for F A here and simplify and we get volume of this equipment is F A 0; what is the entering here this is F A 0 what is the entering what is leaving. So, volume of the equipment is F A 0 multiplied by this integral d X A by minus of r A. Please recognize that we had stirred tank C A 0 X 1 C A 0 X 1 by minus of r A.

On other words, here we have an algebraic equation here we have an integral. So, there is a difference. So, this is the differential equation whereas, this algebraic equation. So, when we have stirred tanks we deal with algebraic equation; when we have plug flow reactors we will deal with differential equation. Let me the equation relates with variables that we change as you change the equipment from one to the other. Now, that we know the size of the equipment we can now talk in terms of what is called as residents time that is defined as volume of the equipment divided by the flow rate flow rate of the inlet. So, the way in is defined as but the residents time is defined as volume divided by the flow rate at the inlet. In other words, saying that use in that this volume flow can change has it flows through the equipment. But, the way it is defined it is defined with respect to inlet flow.

On other words residents time also involves certain reference flows at which we do our calculation its convenient its convenient do it that way. So, if you defined that is way. So, if you defined residents time is V by v 0, then this equation becomes C A 0 this is the known quantity; this integral d X A by minus of r A. What is r A is rate of chemical reaction, this number comes from understanding the chemical kinetics and we will related date look at how we can determine this function that determined this function r A. Now, having said this let us just quickly understand these functions recognize that this volume depends on X and r A.

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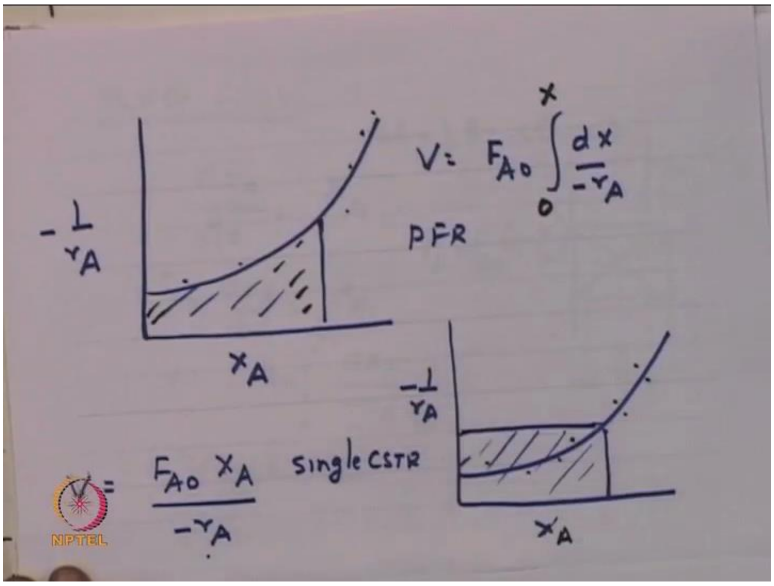

Suppose we plot have you said this suppose they make a plot of one by r A please see this functions X and r. So, if I plot x versus one by r A; you notice that this area this area is what we are taking about. If you look at this you can make a plot of one by r A versus X that is what I have done here one by r A versus X. Therefore, this term X 1 by minus of r A is simply the area under the under this curve this rectangle is the area. So, this area of the rectangle multiplied by F A 0 becomes the volume of the equipment. We can see here if I plot X versus r A as I have done here X r A you can see here this area multiplied by F A 0 becomes the volume of the equipment.

Now, for a plug flow reactor we said 0 to X dx by minus r A. How do this when you plot 1 by r A X A this integral is simply under this curve area under the curve. So on other words, what we notice here is that the way we are formulated the problem of single reaction taking place in ideal vessels; whether it is stirred tank whether it is plug flow the plots of one by r A versus X actually it gives the way of determining size of the equipment. For example, in many cases it may be easier you to determine this function 1 by r A versus X from your experiments the functionality r A may not be known. But data may be available that you may have the experimental data here. You may have experimental data you may have experimental data so that you can use the experimental data and determine what is the size of the equipment?

In many cases particularly reactions, which you all many complex reactions etcetera; you will find it easier term actually make a plot of 1 by r A versus X A. So, that we can determine the area under the curve and hence size of the equipment is very convenient that way and it is preferred most cases you will find this might be much faster way of determining size of the equipment that may be of listed. So, what we have try to say so far is that if you have a batch if you have a continuous equipment like CSTR or a continuous equipment like PFR; you can plot this 1 by r A versus X and then find out the size of the equipment.

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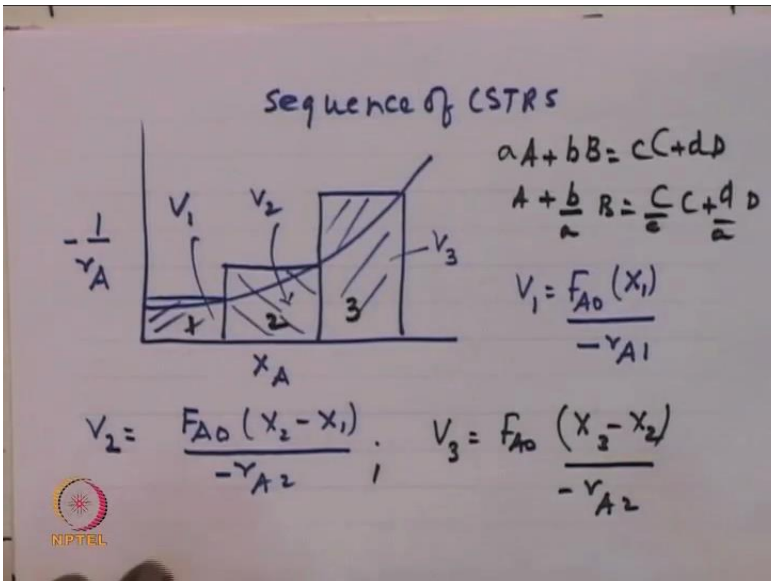

Recognize that support instead of one tank you have many tanks and other words if you have several tanks in sequence by the V 3 is F A 0 times X 3 minus of X 2 divided by r A 2 the minus. On other words, if you have a plot of minus of 1 by r A our reaction once again please recognize that our reaction still this there is no change. We are still looking at single reaction A plus b by a plus B equal to c by a C plus d by a D; we are still looking at this. So, if you have a sequence of tank one so, this is tank one this area this is for tank one; this is the area for tank two; this is tank three. Therefore, size of tank one two and three can be calculated by multiplying area and the curve by the flow F A 0.

So, this graphical procedure gives you a way determining size of the equipment size of the equipment simply by experimental data and that is great advantage of this procedure. Because you do not have to look for a functionality to determine the rate of chemical reaction the huge advantage that is the particularly for the reaction were you have you have great difficulties and understanding that what is going on experiment will be easier another point that frequently that we might want to know is suppose you have continuous equipment continuous equipment that is say.

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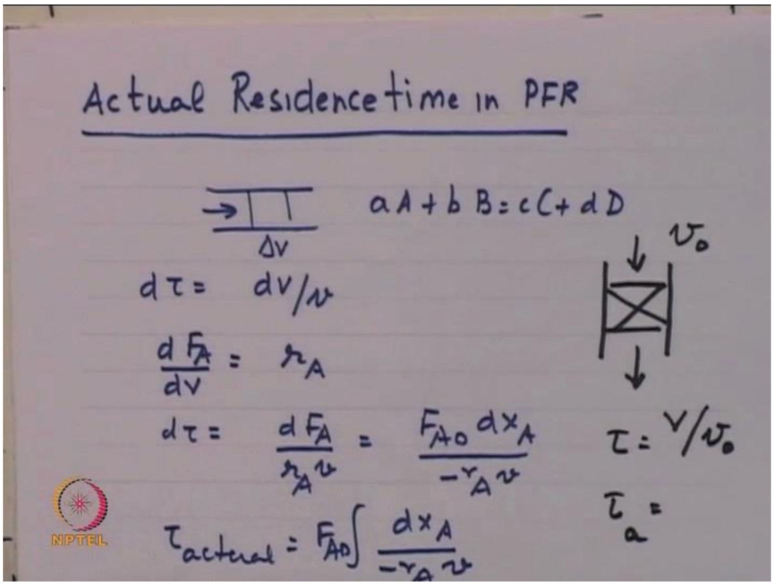

Let us say catalytic for example and due to chemical reaction as you can see here in the chemical reaction there could be some volume change. How do you account for the volume change? We account for this volume change they recognizing that our equation d F A by dv equal to r A; this is the fundamental statement of material balance for a plug flow vessel. We also know let the time of residents is given by dv by v. On other words if you have a plug flow equipment then the residents time at every point is given by dv by v and this is the general statement of material balance by combining these two; now we can tell that what is the actual time of residents after fluid elements inside this equipment. So, what we are trying to put across here is that if you have plug flow equipment in which there is a chemical reaction taking place.

As a result of which there is some volume change and you can take their effect into account through this equation. So, you not only can find out residents time using our residents time can be on the basis of inlet flow; we can do residents time this way or we can do residents time actual which is given by what is this. So, both form both approaches are available and whatever is appropriately you will used in a given application. I will stop here with this we will take up this at in the next lecture; the implication of what I have said for its application to various that we would encountered.

Thank you.