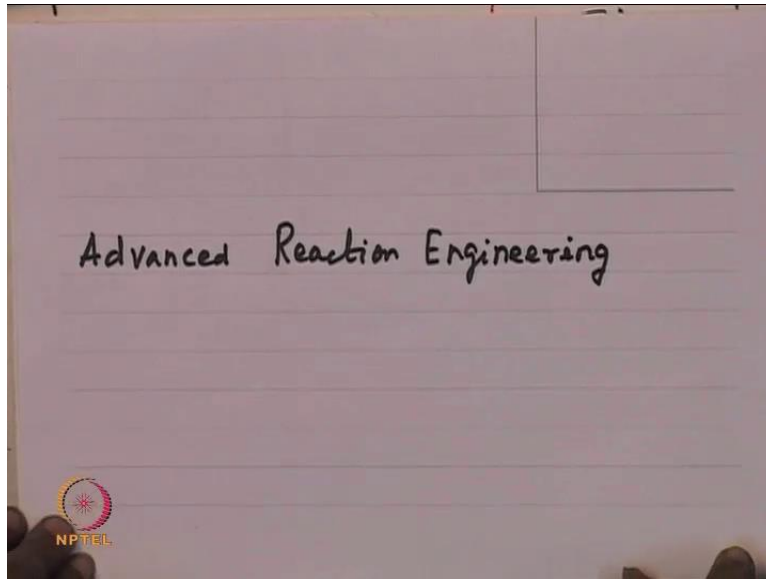


**Advanced Chemical Reaction Engineering**  
**Prof. H. S. Shankar**  
**Department of Chemical Engineering**  
**IIT Bombay**

**Lecture - 01**  
**Course Overview-1**

(Refer Slide Time: 00:21)



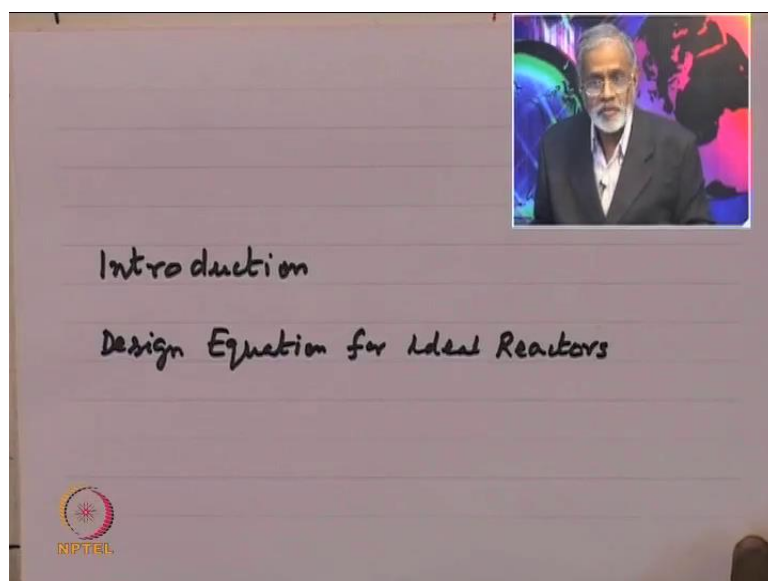
Welcome, this is advanced reaction engineering course. In this course, we covered a lot of ground application of chemical reaction engineering to our requirements in chemical process industry and as well as in daily life and so on. So, what I would like to do in session is, just give you an overall perspective of what I want to do in this lecture series of this may be thirty forty hours. So, let me just run through one by one this gives you a feel for what is contained in each of these modules.

(Refer Slide Time: 01:14)



So, let beginning so we have begun with introduction, I mean the object here is to try and bring to your attention; what we will do in this course of course; and then what is the methodology that we will follow; and how we plan to address various issues; and how we will learn explain the principles through various examples and so on. So, the methodology we will try to drop here is one of problem solving, so that we learn how to derive the equations that describe certain process and or certain idealization that we look at and also show how it implies to different situations. So, that is the way will go around in this course and if you are sure all of you familiar.

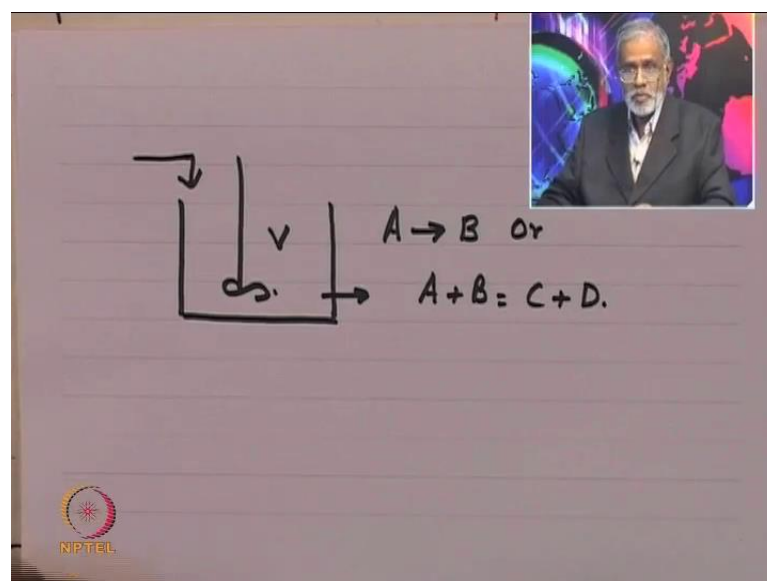
(Refer Slide Time: 02:18)



But, so we will look at what you see as design equation for ideal reactors. Now, I mean you mean in the sense that you know have reaction equipment and that reaction equipment in, which certain reaction takes place. Let us say A goes to B or A goes to B plus C whatever. So, what we need to know is how this particular material is entering reaction vessel; how it undergo reaction; at what extend what it undergo reaction what are the parameter that determine they extend to reaction that occur. Most importantly, what is the size in the equipment that is required for certain extensively action of course, our interest and in some cases you know we are not looking at simply continuous operation. We will be looking at batch operations in which case are interested is to find out, what is the time that is required for given extensive reaction and soon.

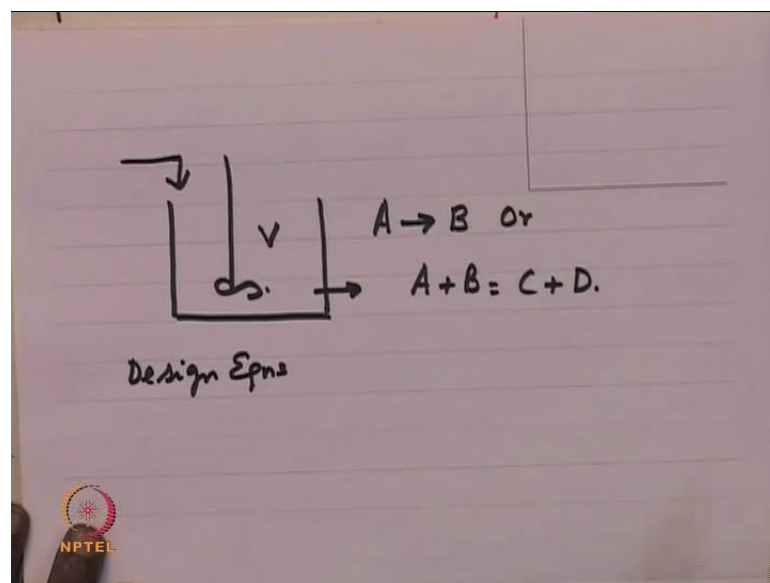
These are situations in which we are, neither doing continuous nor doing batch, are we doing something semi-continuous or semi-batch operations, in which case our interest is to really understand how the process can be written down in terms of mathematics. So then, we can tell what might happen to the process and how we can intervene in a way, so that the process can be made to move in the direction of our interest. So, the design equation for ideal reactors is essentially a way of trying to in terms of mathematics idealize, what might be happening and so that our equation are able to approximate what might happen into our life. Just as an example more of you it will see when you actually look at this just put it in this perspective.

(Refer Slide Time: 04:19)



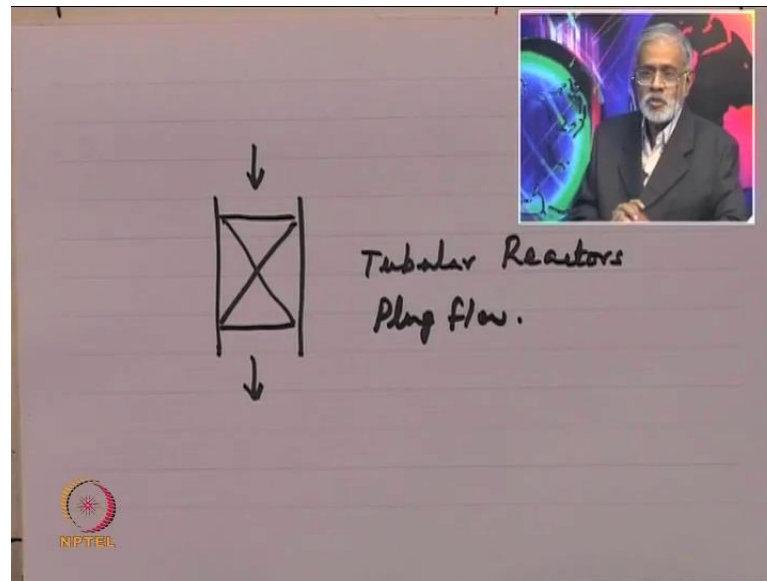
Let us say you have an equipment like this and in which you know this a reaction is occurring flow is coming in and flow is going out; this is got a certain volume  $V$  reaction  $A$  goes to  $B$ . Let us say  $A$  or  $A$  plus  $B$  going to  $C$  plus  $D$ . Now, you will recognize that  $A$   $B$   $C$   $D$ ,  $A$  can be a gas  $B$  can be a liquid you know it can same phases may be different products may have some of it may be a gas some of it. You know various kinds of situations that as likely so far each of these situations in our equations must be able to appropriately in take into account. So, we will look at simple situation as you go along with modified take into account in more variations that may occur in life.

(Refer Slide Time: 05:17)



So, the design equations if we looking at design equations, object of design equation is to put down in simple terms how inputs and outputs or inputs initial and final can be related in terms of parameter that you can understand recognize and so on.

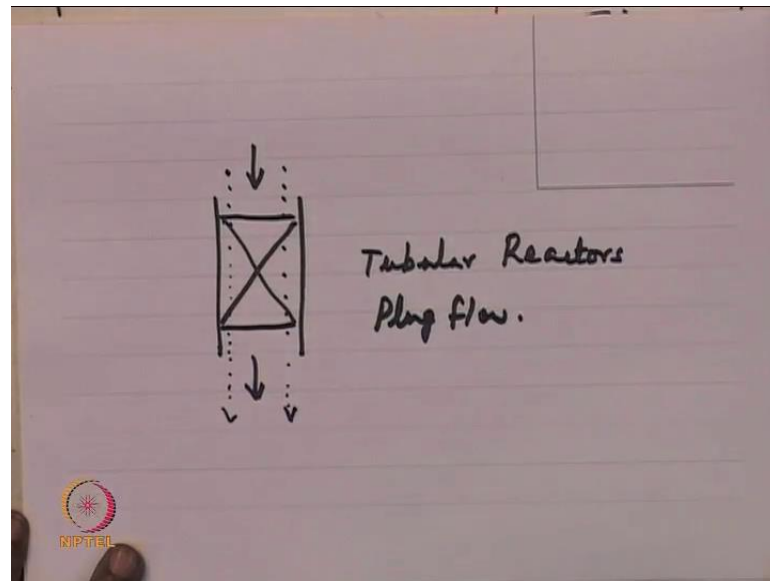
(Refer Slide Time: 05:42)



In the chemical engineering literature or chemical process industry frequently, we see what we call as tubular reactors. Now, tubular reactors are essentially pipes of various sizes and typically they contain a catalyst, which is feed this and going on. Tubular reactors are common in industry; because they are easy to build and then you know flow fluid can be easily understood can be major place. Lot of techniques has been reward numbers of years understand the fluid mechanics therefore; it is common device which is employed in industry.

So, often we talk about plug flow in our tubular reactors design equations the plug flow I mean in the sense the reason, why we idealize situations like this they easier to treat. Therefore, we are able to get equation that is able to quickly idealize what might be otherwise it is difficult to understand and predict so we have first principle to understand.

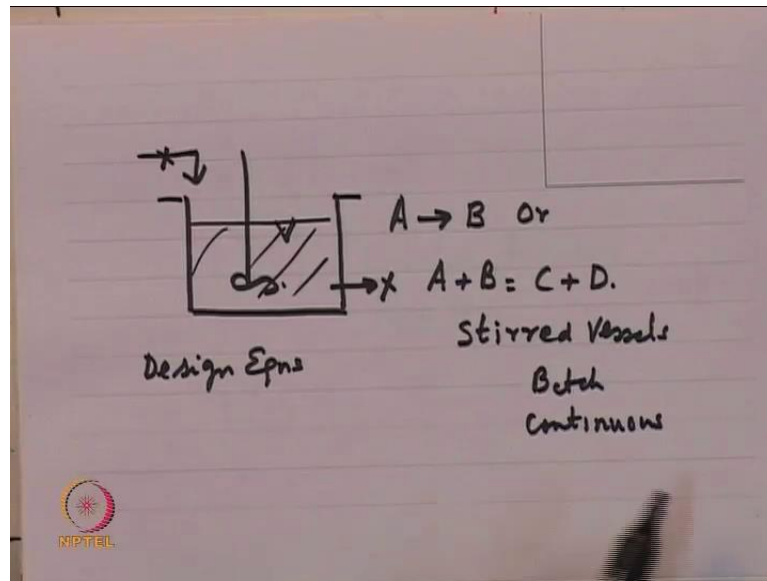
(Refer Slide Time: 06:53)



What might happen by plug flow what is main is that, if we have if you have flow delimit here it sort of get cell it sort of most through the equipment most through the equipment it emerges. In the another fluid element it comes most to the equipment it emerges and other words what we are saying is that if we recognize or idealize flow through equipment as plug flow, it only means that these two elements pass through without recognizing these existing elements.

Therefore, the time of residents of these two elements can be very very precisely calculated and therefore, we are able to tell how long they bend in the equipment. Therefore, we can tell what the extent is, to which the reaction may have taken place based on the numbers that we have in our hand. So, plug flow is idealized version of the reaction equipment that you will see the process industry often we called as tubular reactors. So, we will set of equations we go along to describe what is called as plug flow reactors.

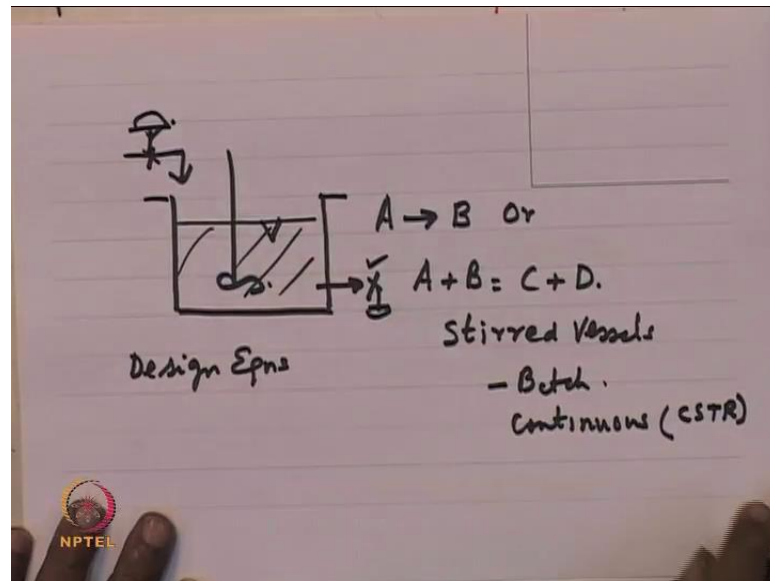
(Refer Slide Time: 07:57)



In earlier, we said we talked about stirred vessels, these are all stirred vessels. Now, stirred vessels cells can be batch equipment or can be continuous equipment. Now, batch equipment means the flow inside, but there is no flow outside in the sense in batch there is no flow in. So, you start with certain under fluid here and we process the fluid in the set of time then, we set of equations that we describe what might be going on inside the equipment. Other words there is no in flow there is no out flow therefore, whatever happens in the reaction is like it is counted for by the process or the reactions kinetics that is responsible for the reactions take place. So, batch you will find batch equipment or then quite common in small scale industry; if we go to paint industry; if we go to pharmaceutical industry or oil industry various kinds of industries whereas you want to process them in small scale.

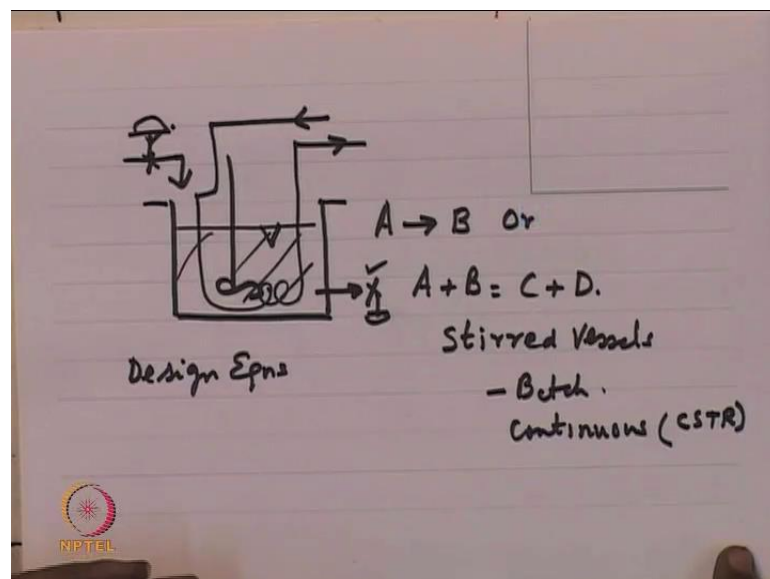
Because, the scale of operations such that the demand such that to small scale industry or precisely pharmaceutical industry where purity and then quality etcetera. So, stringent you must be able to track of in which batch it is produced so that, in case you would not recall the product in next stage it might be possibly to actually inform the dealers to recall the products, in case it is goes to unsatisfactory for whatever reasons. So, pharmaceutical industry batch process is quite common. Now, if the batch equipment is essentially vessel which is got you know the position is inlet and outlet the position for entering inside and cleaning and so on. So, this quite common of various sizes may be ten, twenty five to ten kilo liters typically the size is you will see in the stream.

(Refer Slide Time: 09:58)



Something is called CSTR, which is quite common in chemical literature this is called continuous stirred tank reactor, which is some equipment is like this there is continuous input and there is a continuous output this valves this are the valves so these are open. So, that was continuous flow again and other words what you seeing here is that chemical reactions takes place as the flow comes and goes out.

(Refer Slide Time: 10:23)



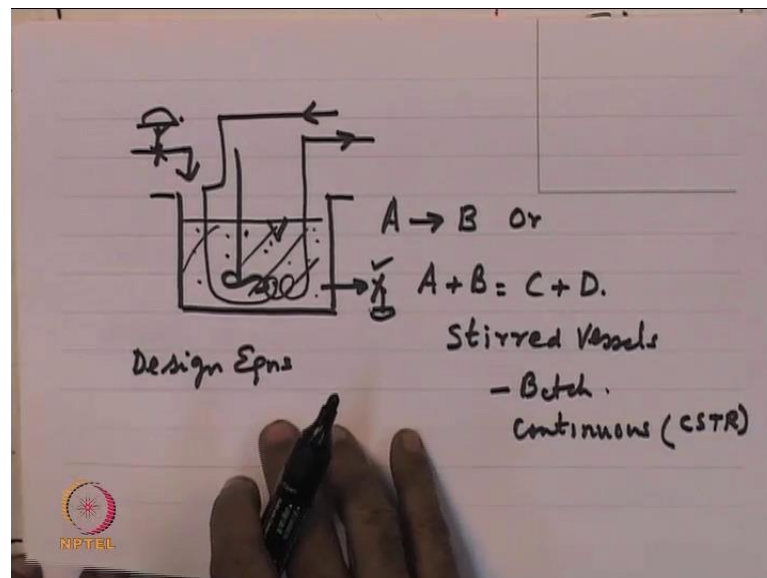
And since many of the reactions are could be quite in exothermic, there are quite there is which might be carrying heating or cooling fluid so as to ensure the reaction condition



can be able to be achieved because this heating or cooling media. So, the continuous stirred tank reactor is very common device that you may see in laboratories in the universities and research labs and the industry, where the scale evaporation are relatively larger not very large relatively larger; now continuous stirred tank reactor in the process industry in common we might see in places.

For example, you will find that in polymer industry where you are deal with very viscous situations then you find that stirred tank provide good amount of mixing and so on and heat transfer can be satisfactory. You will find continuous reactions equipment in chemical in polymer industry. There was some situation where continuous reactions equipment is quite common because in fact, permits you to continuous input and output at the same time ensure the temperature and process conditions and kept uniform. So, CSTR and batch are stirred equipment that you will see in the process industry and the tubular reactors are plug flow devices that we called is quite common in the very large scale petroleum and other industries. So, for both these both these situations are there are design equations which we call as ideal reactors.

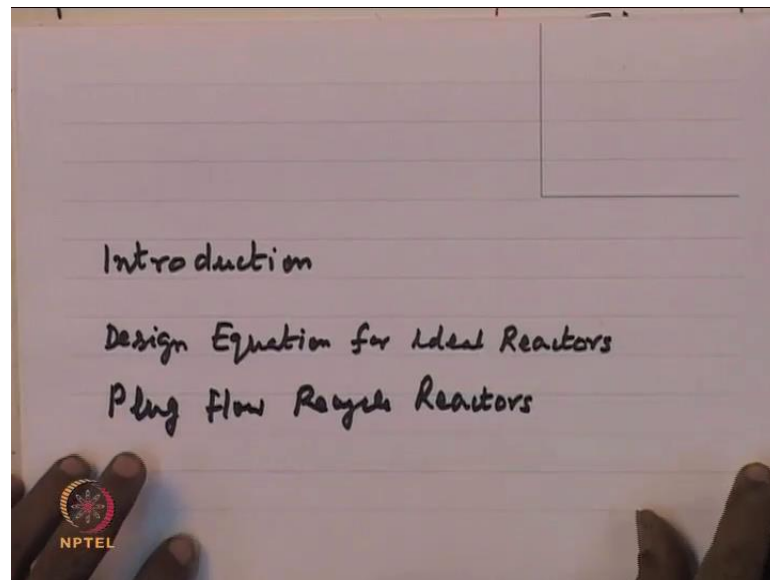
(Refer Slide Time: 11:59)



So, what is meant by ideal reactors by ideal we mean that the condition the different parts the equipment, in terms of temperature pressure concentrations are uniform in other words the flow that enters it is able to get mixed. So, that the conditions inside the equipment is same as condition that leave in the equipment this what is called continuous

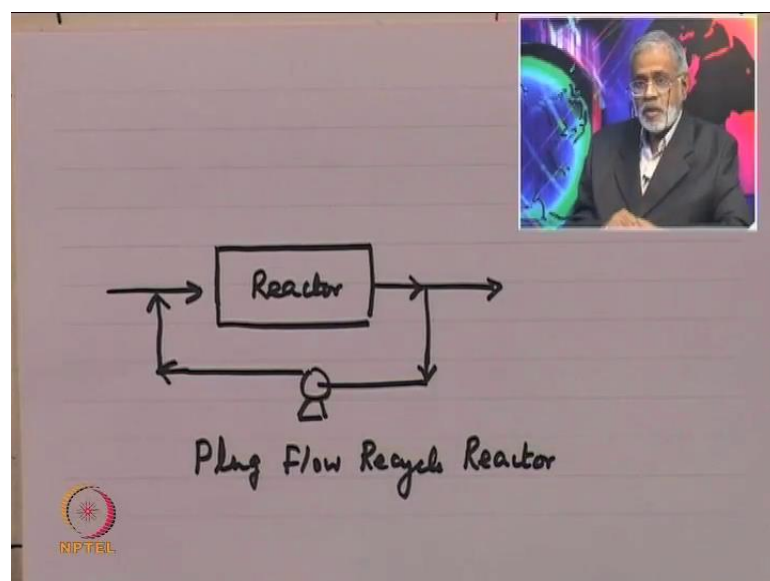
stirred tank reactor, very popular in the chemical reaction engineering literature. So, when we when we said design equations for ideal reactors we will be looking at these two situations and set of equations that will describe how reactions takes place in these to how reactions can be we understood as they take place in these two kinds of equipment.

(Refer Slide Time: 12:42)



We find in our experience in our process industry that the reaction does not go to completion so, what do we do.

(Refer Slide Time: 13:09)

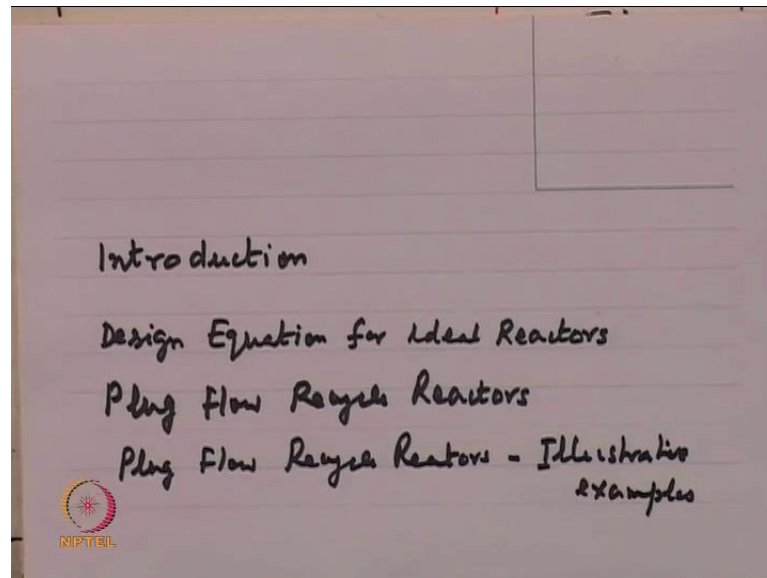


Let us give an example. Let us say you have reaction equipment its coming in and it is going out. Now, we find that this is the reactor this is what is called plug flow plug flow recycle reactor. Now, when would be process we would engage process at this nature when we find that the products that come out of these reactions request to be inside that would be situation you will learn as along situations in which products that be recycled that would be recycled. Because, you find that the products are able to facilitate they needed with reactions occur is could be on reason or the products contain lot of energy like heat for example, is very high temperature.

So, you make use of that energy for your process like could be another example. So, there could be several situations of course, another example could be that you know the reactions cannot as in completion. Therefore, you want to put separate somewhere here and then separate the products and recycle the reactor products. So, there are various situation you will encounter recycle is required. Now, will recycle is required need to set up our desired equations, which will take into our account the effect of recycle the effect of recycle on the size of the equipment number one effect of recycle in extensive action, there were some issues that we must consider when we provide recycle; it can be steady state or it can be unsteady state.

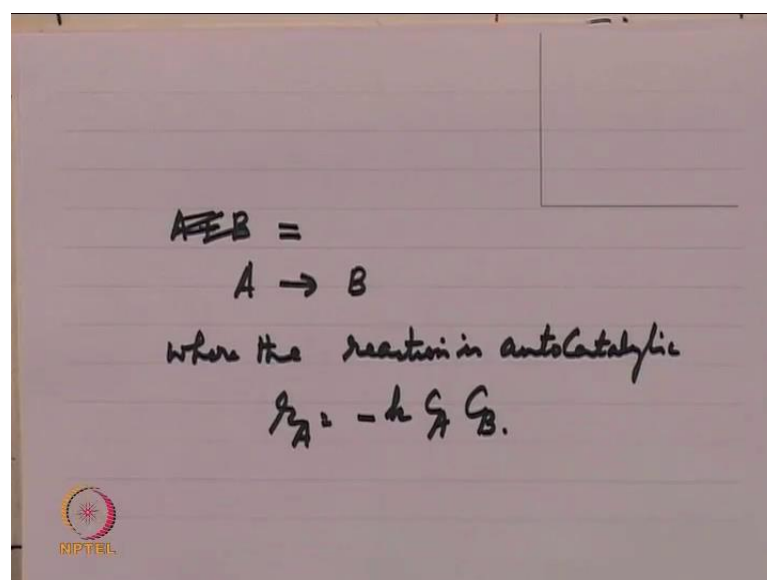
Because, you know you might be encountering situations then which you also want understand how long it takes for certain process to reach steady state or you are interested in unsteady state part of the process. Because, you are starting of the process and you want to know how long it does taken to reach steady state, various issues that may come up in a process that you would like to understand and then set up or mathematics So, that we can actually tell how long it will be before the steady state is achieved. So, we meets situation like this in process industry. So, you will set up equations that take into an account the effects of recycle so that, we can set up the equations appropriately.

(Refer Slide Time: 15:54)



I will set this you want to look at plug flow recycle reactors. So, illustrations illustrative examples now what you will when I say plug flow illustrative examples. What I would like to bring your attention to in such lectures what are the physical situations where you might want to do recycle and how that recycle benefit you in a process lets taken an example.

(Refer Slide Time: 16:37)

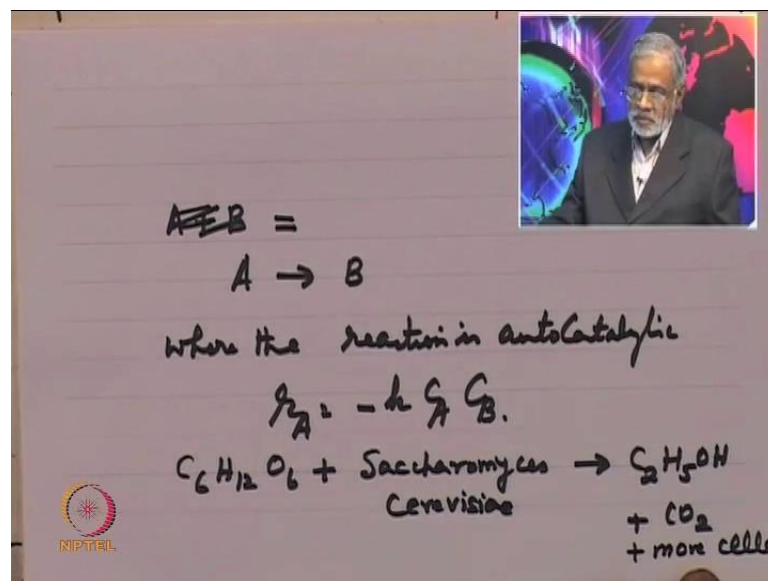


Say for example, A tend to B let us take an example, where the reaction the reaction is autocatalytic is autocatalytic; what is mean by autocatalytic? You mean that the reaction

A that reaction occurs is depending on A it also depend on B. Now, when reaction is autocatalytic which means that the rated which the reaction moves only depends upon how much the products is been put into the system. So, clearly speaking and you put product appropriately the reaction does not move. Now, if you look at the recycle this recycle device provides a way by which you can put the products back into the fluid. So, autocatalytic reaction is a good example why the recycle becomes very very important for the process to move forwardly.

So, autocatalytic reaction require recycle and very clearly it will they might be optimum recycler which you must operate and so on, which is important from the point of your process of variation all these features will have to be appropriately taken into account design equations plus it has to be appropriately explained when we look at illustrative examples now. If we look at real life for example, what are the real life situations where we have to deal with autocatalytic reactions the finest example you will think of or biological reactions.

(Refer Slide Time: 18:19)



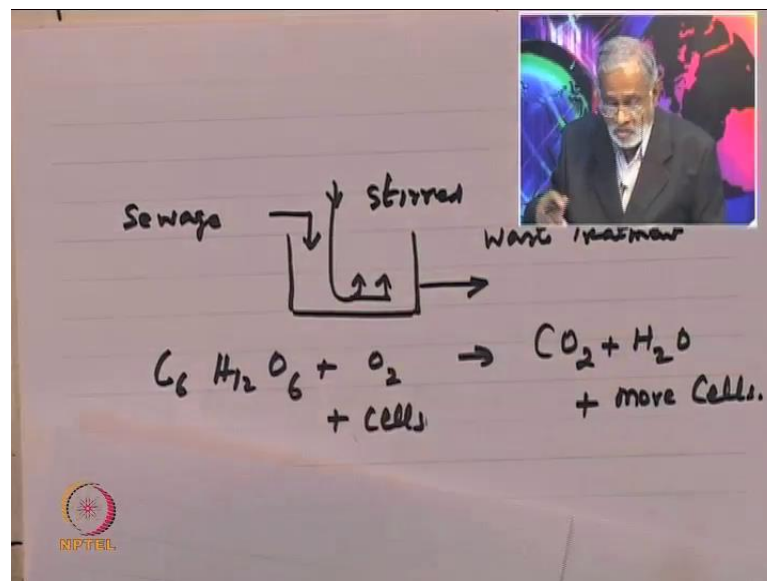
$A \rightarrow B =$   
 $A \rightarrow B$   
 where the reaction is autocatalytic  
 $r_A = -k_A C_A$   
 $C_6H_{12}O_6 + \text{Saccharomyces Cerevisiae} \rightarrow C_2H_5OH + CO_2 + \text{more cells}$

Say for example, you have let us say we have let giving a small example we have from C<sub>6</sub>H<sub>12</sub>O<sub>6</sub> this is glucose; it is reacting with some cells. Lets us say, saccharomyces cerevisiae this is fungi which fluid on glucose under certain condition with pH and temperature and oxygen tensioning and so on, gives you alcohol it gives you alcohol and carbon dioxide. Now, you can see here is three C<sub>2</sub>H<sub>5</sub>O<sub>2</sub>H and C<sub>2</sub>O<sub>2</sub> you can balance

this how many carbon is there. You can balance this anyway this is not so critical right know. So, you have glucose giving you alcohol and water and carbon dioxide. Now, this particular reactions you will find that unless you put saccharomyces and get the appropriate condition you will not able to produce alcohol.

So, what is being said is that so the presence of saccharomyces mixed reaction happen in that process more cell are formed. So, in principle these cells can be harvested and then put back into the process. Alternatively, you find as more and more cells are formed it is able to catalyze the reaction in forward direction. So, autocatalytic this is the good example in which you will find that the addition of the products which cells of the product and enhances rate of forward reaction let us look at some more examples of recycle reactors. Now this another situation that you would have seen in real life in some of may have seen is if you go to the waste treatment plant see if you I mean all over the world.

(Refer Slide Time: 20:17)



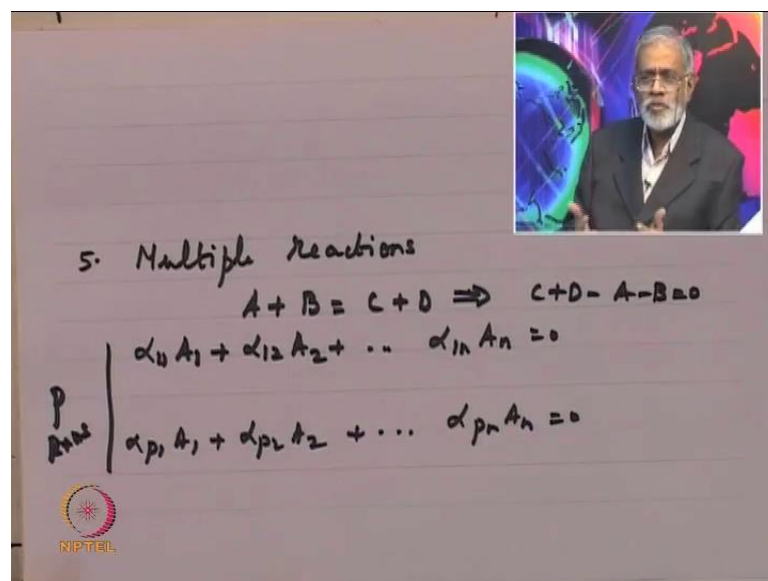
You will find that we produce lot of sledge say sewage which comes out of human settlements; there could be waste coming from daily sledges which contains lot of waste materials. So, typically what is done is that these materials is taken into a basin in which you know you put an oxygen you put in oxygen by aeration and then presence in the presence of oxygen and the sewage, which contains organics like carbohydrates and things like that. These cells which is present in the environment grows and as a result

you will find the waste material and consumed and water that comes out is relatively or this is called as waste treatment this is called waste treatment.

You will find you will find that that sewage let us say sewage contains carbohydrate you have put into oxygen. So, this gets oxidized. So, it get becomes carbon dioxide and water and this cells are present in the water to produce more cells. So, this is the another example this is the another example where the whole reaction course forward only if there are cells and the cells produce more cells and effect of the cells is to further enhances reaction. On other words, this is very good example of autocatalytic reaction. Now, whether you used devices we can use various types of devices. We can use devices which is called stirred tanks which is called these are all stirred tank; we can use stirred tank device for doing this process or you can recycle the devices that what you have said.

In both cases the principles are that in the product which is sell enhance the rated which the reaction occurs, this is what we are trying to say. So, plug flow recycle devices are recycles are general are very common in chemical process industry and we need equations to take care of how to deal with recycles in real life in that is what we will do in this kinds of lectures. We know often find this mean this is very unusual in chemical process there are many many reactions that occur there are many many reactions that occur.


(Refer Slide Time: 22:43)



5. Multiple reactions

$$A + B = C + D \Rightarrow C + D - A - B = 0$$
$$\alpha_{11} A_1 + \alpha_{12} A_2 + \dots + \alpha_{1n} A_n = 0$$
$$\alpha_{p1} A_1 + \alpha_{p2} A_2 + \dots + \alpha_{pn} A_n = 0$$

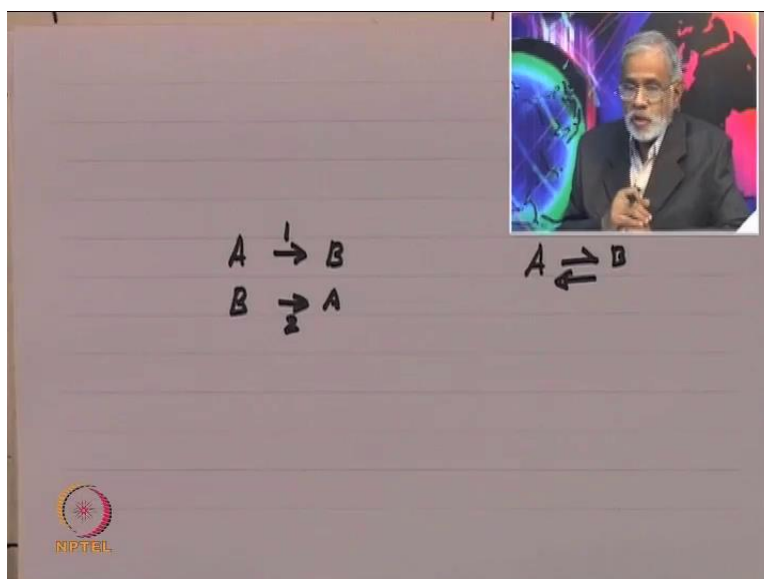
*P*  
*Rows*



We have to deal with what is called as multiple reactions multiple multiple reactions what do you mean by multiple reactions? What we want to say here is that suppose let us say just for an example, I write  $A + B \rightarrow C + D$  this is the reaction. Now, if you want to talk about multiple reaction, I can write the multiple reaction like this  $\alpha_1 A_1 + \alpha_2 A_2 + \dots + \alpha_n A_n$ . Similarly,  $\alpha_{p1} A_1 + \alpha_{p2} A_2 + \dots + \alpha_{pn} A_n = 0$ . What is being said here that we have  $A + B = C + D$  as the reaction can also be written as  $C + D - A - B = 0$ . What is meant is that chemical reaction you can write it as algebraic equation its convenient. Many many reactions occurring as I said one  $\alpha_1 A_1 + \alpha_n A_n$  as this is one reaction there are  $p$  such reactions. So, there are  $p$  reactions here.

Now, the important point is when there are large number of reactions are happening. So, we also like to know I mean how to manage; how to understand with large number of reactions. Now, therefore, we need a systematic procedure by which we are able to deal with very large number of reactions. So, that we can confer them we can find out what is what is happening in the reactions and so on. So, the general technique which is used to understand how many reactions are independent knows. Independent reactions is an idea which coming because of the factors there are many many reaction happening. Once we recognize what is called independence of reactions; we can also understand that if there are many many reactions how many of are them independent; how many of are them dependent and so on.

(Refer Slide Time: 24:53)

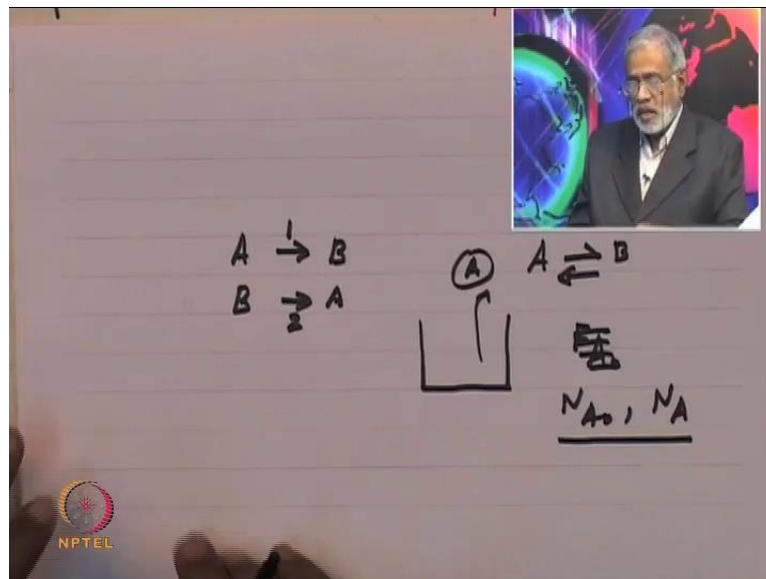




Let say illustrate this, what am saying say for example, reaction A going to B and reaction B going to A. What is meant by this? You are saying that this reaction A is to B is this is a reversible reaction; that means reaction going forward direction or going in reverse direction. So, which means when we are conducting a reactions A going to B in principle perhaps both the rate processing occurring. What we see is that the reaction goes to A to B because on rate processing faster than the other. Therefore, the net in the net you see that the reaction going for one direction. There are technique I mean you have learnt or you will learn as you go along by which actually measure the rate processing directions.

There are techniques available; there are methods available; you will learn all these as you go along. Therefore, in principle all these are possible to measure so, but the fact of interest of that if there are there are A going to B and B going to A. How many of these reactions are independent that the question that we frequently asked?

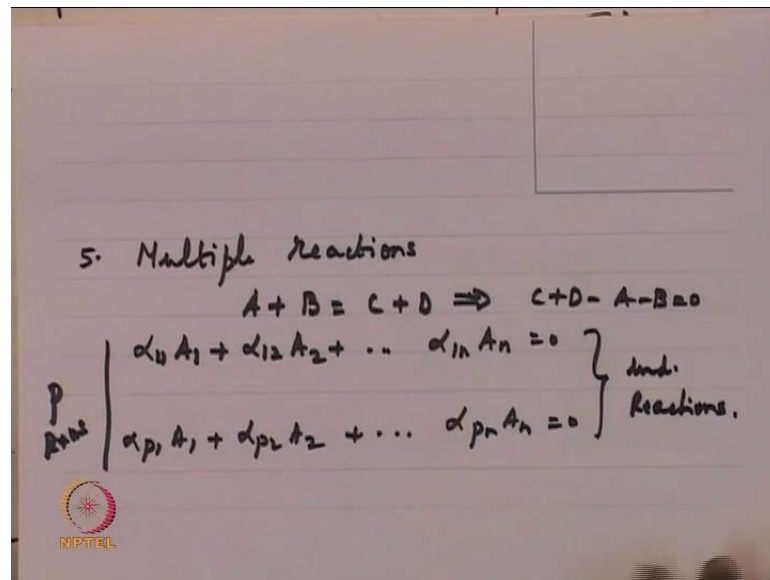
(Refer Slide Time: 26:10)



Now, it is common sense by looking at we can say that if just take one sample of suppose this reaction occurring in the equipment like this A going to B;B going to A. We just going to take a sample of A this of this material and analyze for A if you analyze for A A zero is total moles and then we determine what is the moles at any other time. So, once you know this difference once you know this difference you can tell what is the amount of B? that is formed because that is coming first tachometry. In other words what are

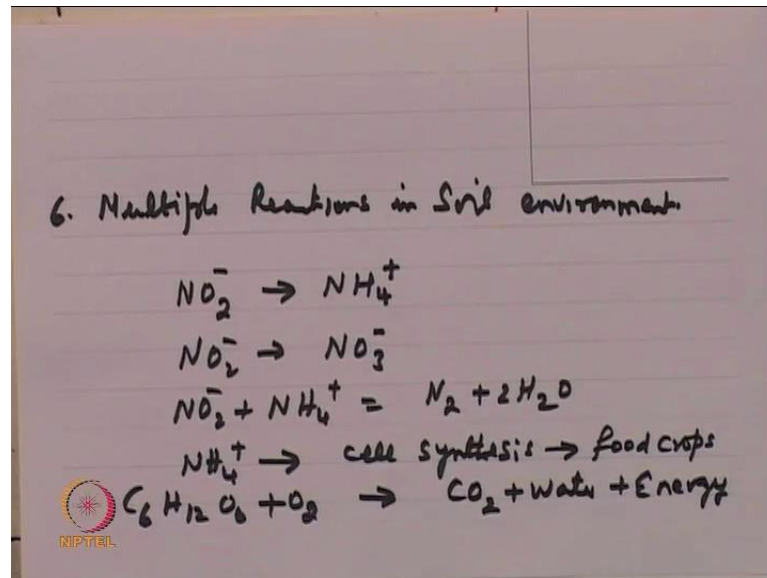
trying to say is that if you know that independent of reactions you can tell what the composition of the system is? So, what is what is generally jested in multiple or it was called as a reaction network is that we determine we determine the number of independent reactions.

(Refer Slide Time: 27:00)



We just tell that that number of independent reactions. Once we know the number of independent reactions; we can we can tell the compositions of the system fully because that is what determine the compositions of the system. Then as you go along you will use this general methods to deal with multiple reactions and you find as you go along particularly biology huge number of reactions occurring infinite deal with use this techniques. Because it makes very convenient and there are computationally methods available so, which we can deal with very effectively. Now, I will set this set this let me sort of attention to very very interesting situation we make in counter situation, which we will is multiple reaction.

(Refer Slide Time: 27:54)

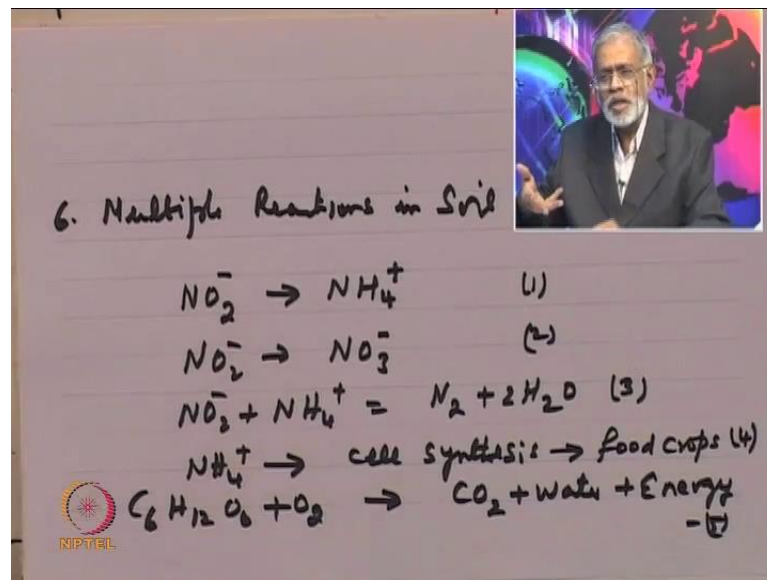


Multiple reactions in soil environment, if you all know that just give a small example just put this in context suppose you have a reaction  $\text{NO}_2^-$  giving you  $\text{NH}_4^+$  plus so,  $\text{NO}_2^-$  giving you  $\text{NO}_3^-$ . So,  $\text{NO}_2^-$  reacting with  $\text{NH}_4^+$  gives you  $\text{N}_2$  plus  $\text{H}_2\text{O}$  one two three; then could also have a situation that  $\text{NH}_4^+$  which is formed reaction one goes for cell synthesis. How does it happen? This ammonium nitride is actually called cells due to some reaction that happen in soil environment of course, you could also have a situation that carbohydrates gets oxidized to give you carbon dioxide and water plus energy.

So, the context here is something like this I mean this in this planet produce to close to about two billion tons of grains to feed this population of the world. All this comes about thirteen hundred million hectares of cultivated lands different parts of the world India included and the cultivated land. Then India is something like out of total land about 180 or 200 million hectares is the total cropped area in this country. So, in the sense that if you want understands that what is happening in the soil environment?

We can understand this by looking at these five reactions. Now, we can do experiments to find out what happened to  $\text{NO}_2^-$   $\text{NO}_3^-$   $\text{NH}_4^+$  plus and then carbohydrates can we measure appropriately. In other words we can do a small experiments to find out how these nutrients  $\text{NO}_2^-$   $\text{NO}_3^-$   $\text{NH}_4^+$  plus and then carbohydrates actually channel into path ways through simple experiments.

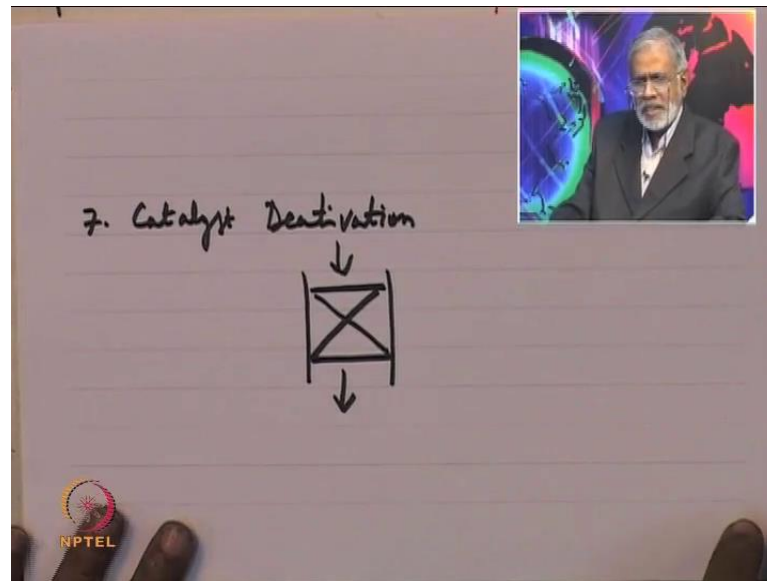
(Refer Slide Time: 30:39)



Now, notice here this is what this is called reaction 1 and reaction 2 call this reaction 3, call this reaction 4, call this reaction 5. Essentially, what we are trying to say that here are five reaction and these five reactions are able to tell us how you are producing various cells it can be food crops or in around the world. So, through some simple experiments I mean in the kind of power that these experiments have an enormous as you can see. You can do this experiments in find out how the nitrogen that we add that we add to soil and how they related to production of food crops and how the carbohydrate that might be present in the soil environment is used for the production of food crops.

These kind of inter linkages we can understand by doing some simple experiments in multiple reactions using soil environment in a laboratory do not have to going into the field. We find that you are able to get results which able to explain what happens in the whole parts of the world they feel for how simple experiments done in the laboratory which does not cost a lot. It gives your insight into very very complex lets happening in agriculture plantations plantation crops in the world and so on.

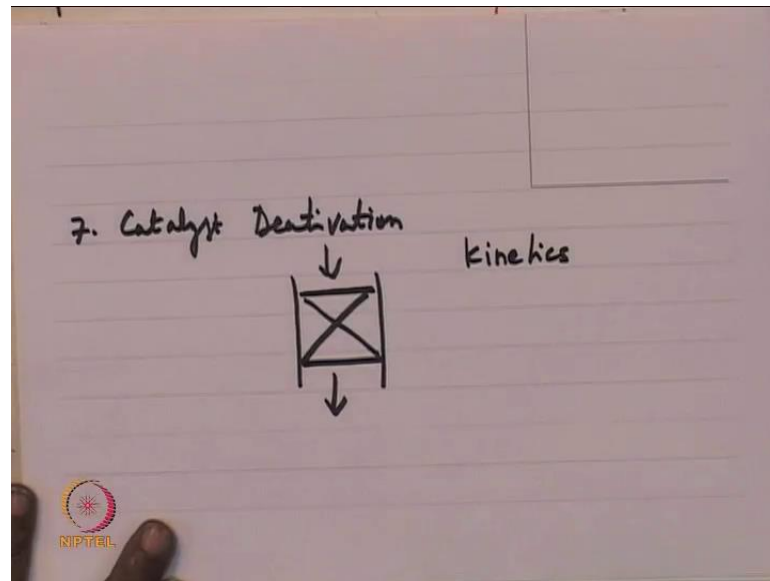
(Refer Slide Time: 32:15)



That is the power of trying to understand in multiple reactions in soil to often you will look at some example to illustrate how we can get insight into fairly complicated situation using fairly simple techniques. Next we will try to look at is what we called as catalyst deactivation. Now, the context looking at catalyst deactivation is that if we look at our process industry our process industry many of them many of them require catalyst for the reactions to take place; I mean we know of ammonia synthesis of which Heber Nobel prize in nineteen fifteen for the development on discovery of synthesis catalyst of course, lot of improvements at comes in end.

There are in fact, catalyst is this centered of many many important processes, which makes life so easy for us today compared what it was may be hundred years ago. So, but catalyst undergo deactivation methods of deactivation as chemistry that we must know that we can prevent it and improve it and so on. But, from point of view of chemical engineers of processes what is important we would like to know what is the kinetics of catalyst deactivation at what rate they can deactivate. So, that we have some way for understanding how long our catalyst will last in the process environment; we can replace them alternatively we can regenerate them appropriately.

(Refer Slide Time: 33:44)



So, the whole process of catalyst deactivation requires you to find out methods by which we can understand kinetics of deactivation kinetics. So, you must know the kinetics deactivation I mean for which you must do measurements and even if you do measurements what is important that we must know how to use measurements to derive and to get the kinetics information of our interest. So, what is important in catalyst deactivation is able to develop our mathematics to represent what is going on in the process so that we can get the information of our interest.

So, in these lectures in catalyst deactivation what we are trying to emphasize and give you methods and do we conduct our experiments. So, that we can get data in a form we can use to extract the deactivation kinetics from our experiments. So, this is the content of the catalyst deactivation that we will do in these lectures.

(Refer Slide Time: 34:45)

7. Catalyst Deactivation

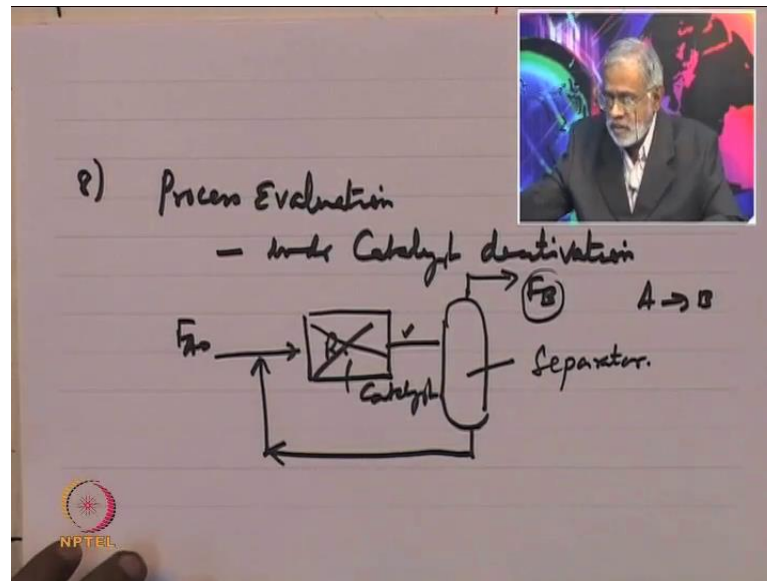
kinetics

$$r_d = k_d a^m f(c)$$
$$-\frac{da}{dt} = r_d$$

The slide features a central diagram of a reactor, represented by a square with an 'X' inside, with arrows indicating flow in and out. The text is handwritten in black ink on a light-colored background. An NPTEL logo is visible in the bottom left corner of the slide.

Now, if you know if I say catalyst deactivation kinetics is given by equation of this form equation of this form some function of concentration and so on. So, our important thing is to recognize is to recognize that what is the value  $m$ ; what is these function, which depends which determines deactivation kinetics. So, that when we write the rated which the catalyst deactivates by this kinetics we are able to convert this in appropriately integrate this to our design. So, that we are able to understand how this process and catalyst deactivation will run. So, that appropriately tune the process to take care of the deactivation and ensure that we produce products the rated that we design we have design the plan for. So, the object of this particular this side of lectures is to determine the function. So, that we are able to go forward and use this information for our design operation and control of processes involving catalyst. Now the related issues which are must bad in mind.

(Refer Slide Time: 35:57)



But I call here as process evaluation process evaluation under catalyst deactivation. Now, what we try to learn here is that let say for example, let us say we have a reactor and let us say it goes through a separator products come out and then reactor this is this is reactor closed pack. This is the most common that we will see in the reactor this is separator. Now, I call this is  $F_{A0}$  if I call this  $F_B$  then example A tends to B. Now, what we will see in a process that as this catalyst; this is the catalyst here this is the catalyst here catalyst which deactivates here this deactivates.

So, what you would expect as this deactivates the amount of products that we will produce here will keep on decrease here. Clearly, which means the amount of product that formed here is decreases in therefore, what we are going to get also decreases. Now, this separator has been designed to process a certain amount of the product. Now as this keep decreasing you will find this this separator is not working to your design. So, it is sub optima and therefore, your process is not satisfied clearly when you design this reaction equipment we have to anticipate what is the deactivation you have to anticipate we have to anticipate the effects of this deactivation A is the activity.

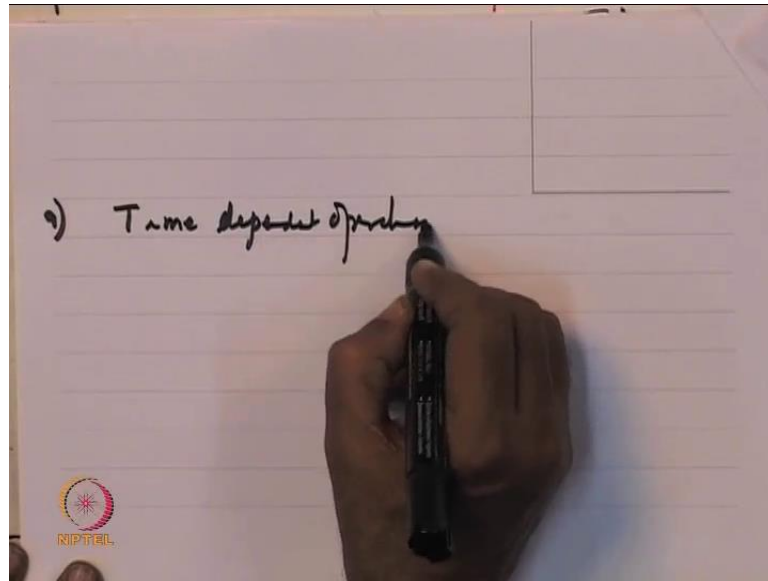


(Refer Slide Time: 37:57)

The diagram shows a process flow starting with an input stream  $F_{A0}$  entering a reactor. Inside the reactor, there is a catalyst bed. The output of the reactor goes to a separator. From the separator, a product stream  $F_B$  is shown, with the reaction  $A \rightarrow B$  indicated. A feedback loop is drawn from the separator back to the reactor inlet. The equation  $r_A = k(A) f(C)$  is written below the separator, with an arrow pointing to the  $f(C)$  term. The text 'Catalyst deactivation' is written above the reactor. The word 'Separator.' is written next to the separator. In the top right corner, there is a small inset image of a man with a beard and glasses, likely the lecturer. The NIPTEL logo is visible in the bottom left corner of the slide.

Appropriately design your process, which means which means rated which component A that is formed let us say this is some this is the activity change with some other function. This effect you should account for in the design. So, that with time with time as this catalyst activity keeps on decreasing there might be must be process tuning that we will do our process adjustment that you will do which will ensure that the catalyst even though deactivates that product that comes out here this is not change with time. So, in other words there are strategies by which we can run processes despite the fact that is deactivation and these strategies that we will learn in this lecture and we will illustrate this through examples where you can actually determine used this principles to understand how we can run this processes.

(Refer Slide Time: 39:24)



We pointed out that commercial process like deactivating catalyst we need to continuously adjust the process condition that the quantity materials that are produced here that unit time etcetera is variant with time; so that we are able to produce these products. So, essentially these are all time dependent kind of operations. So, time dependent time dependent operations. We just now pointed out that catalyst deactivation is an example of time dependent operation and we also said there are strategies by which we can manage this time dependent operation appropriate adjustment of the process condition. So, that the output does not see a time dependents see these are the kinds. Now another set of situations in real life where actually there is time dependency.

(Refer Slide Time: 40:19)

Time dependent operation

(1) Batch process

(2) Start up.

$A + B = C + D$

$t = 0$   
 $C_{A0}$   
 $C_{D0}$

NPTEL

That means, we accept the fact; there is time dependents and we want to be able to understand those time dependents mathematically, so that we can set up our equations. We have all the numbers in front of us therefore; you know how the time dependents actually happen how we take that into an account. So, time dependent operation are one you have a batch process batch process; what is the batch process you have a reaction happening here and then put in at zero time at time  $t$  equal to zero you started with some components  $C_A$   $C_B$   $C_D$  product  $A + B$  goes to  $C + D$ . Therefore, this tells you how long you must run this process so that you can get your products.

So, that is one elementary examples of time dependent operation there is more involved time dependent operation you have let us say reactor, which is to using products now this particular reactor. We have to there is a start up of this what is meant by start up? You have reaction you have a reactor which you are starting now you would not know how long it takes to reach a steady state and so on. Therefore, during this startup up to reaching the steady state there is some time gap. What is the time line; how do we understand the time line and how we ensure during the process of starting up to the point it reaches steady state; everything is very safe that is go on out of control.

So, start up of the plant start up of the reactor is based on time dependent. So, the effect of time must be appropriately counted and incorporated in the mathematics. So, that you know how the evolution of the composition of the system is dependent on system

parameter etcetera. So, time dependents start up is good example of time dependent operation and further matter all start up you know am not this chemical reactor alone you will find that any start up. You have you have to deal with time dependents and therefore, your mathematics take into account all the concerns let me determine the time dependents of a process.

(Refer Slide Time: 42:28)

Example

$A \rightarrow B$

CSTR

Start up time  $C_{Ai} = \checkmark (C_{A0})$

= time required to reach steady state

Let us just take an example to illustrate what is saying. So, what happens suppose you have CSTR a reaction taking place a reaction is taking place. Now this this is an example this mean that they happen in daily life or an industry, but something helps us to understand how mathematics help us to get a feel for what happens and mathematics help us to tell how we can prevent many of difficulties you may typically face if you do not formulate a problem in mathematical terms. For example, this is the instance of stirred tanks called CSTR.

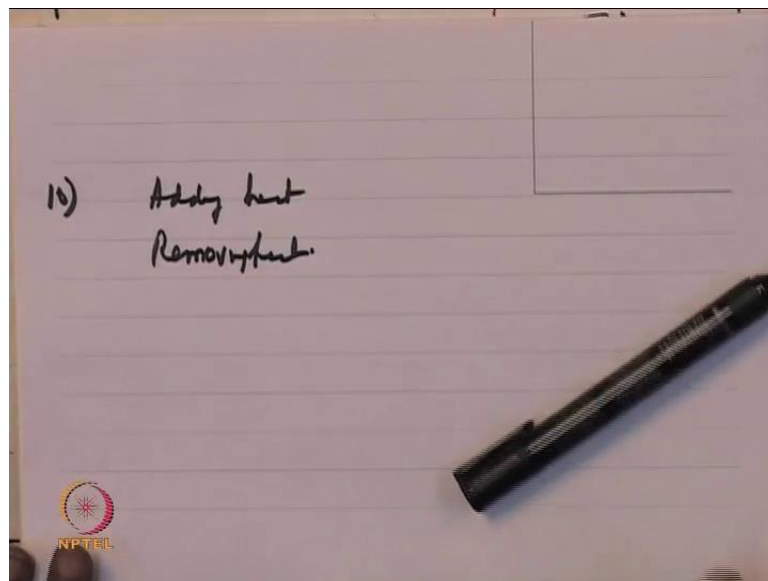
Now, we start this CSTR with initial condition  $C_{Ai}$  this is the initial condition  $C_{Ai}$  equal to some value. I will call this  $C_{Ai}$  into some value  $C_{A0}$ . Now, you will realize by formulating the mathematics that if you choose  $C_{Ai}$  appropriately carefully then the start up the start up time what is meant by startup time? The time that is required for the process to reach steady state start up time is the time that is required time required to reach steady state reach steady state? Now if this required time required to reach steady state is very large you see; then clearly you see you are not the process doing

anything useful for you and whatever you produce unsatisfactory does not recycled anyway so, its that you are endlessly incorrect.

So, if you can keep this time very small very advantageous and your mathematics will tell you how to do it these are the advantageous of being able to formulate the problem mathematically. Because, lot of the answers that you would learn through the experiments through it come through this and save time save cost plus huge insight what is going on this process; something that it gives you a great confident of how to deal with other wise difficult situation. This confidence what might be important in landing processes designing processes managing crisis managing safety issues and so on.

So, this is important part that we will try to illustrate through an example to say how start up how the initial state that you can chose so that we can keep this start up time as small as possible now what we are try to do in the in the lectures of seven eight lectures. You should set up the basic foundations of for dealing with chemical reactions and then setting up the equations required to explain what is going on. See, we have so far talked about situations where the system has been assumed to be at constant temperature when we are counted for effects of temperature in the process. Now I mean am sure you are recognize this chemical reactions typically releases heat or requires heat.

(Refer Slide Time: 45:45)

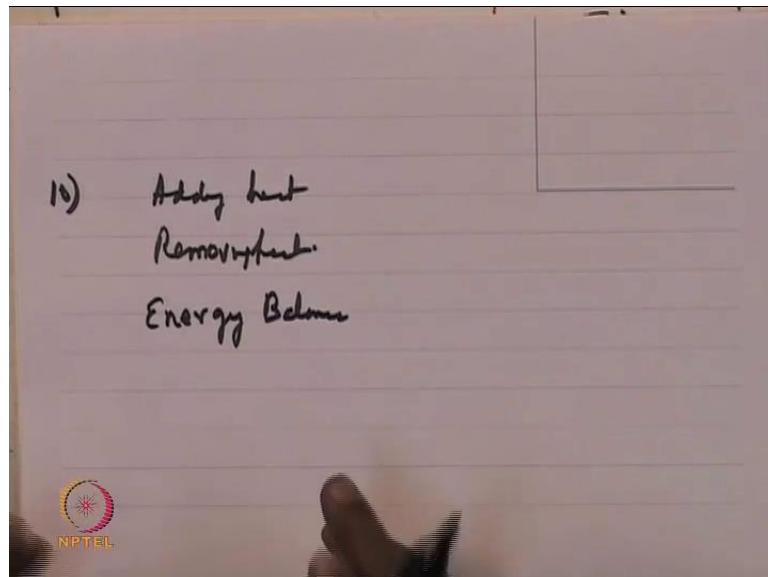


So, adding heat or removing heat; heat are two important situations that we all have to account for so adding and removing heat crucial to managing chemical reactions and

giving small example I mean it is not that is known about. Suppose, you are looking at power plant in which burning coal to make steam as an example. I mean Coal combustion is very well studied chemical reaction is huge amount of energy, which we use to make steam then the steam is used for turning turbines and make electricity and so on.

Now important thing is that that the rate which the coal is burning and the rate which the steam what are the going through the can able to pick up the heat and then converted into steam and then you have to match the two. So, the rate of combustion must be equal to rate of production of steam. So, that design these are the kinds of design features that you are look into when we are looking at chemical reactions.

(Refer Slide Time: 46:49)

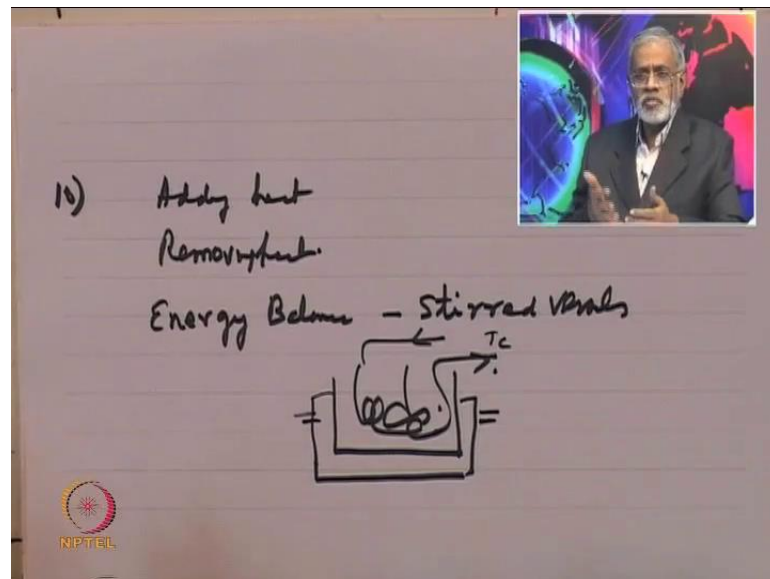


So, energy balance so what we are saying that energy balance energy balance is crucial for reactor design crucial to reactor design, which means you must take into an account whatever energy is going into the process; whatever energy is coming out of the process and the energy that we are putting into the process might be in the form of internal energy. Well, energy is coming out of the process might be in the sensible heat you have to see how the energy of internal energy or enthalpy as you can say is actually used in the process. Therefore, we have to see how heat is generated because of chemical reaction how heat coming out of the chemical reaction can be appropriately channel into the process and so on. So, energy balance is crucial to understanding how reactions take

place; but reactor design actually requires not just understanding the material balance of talked about so far.

But requires an understanding how material and energy balance are connected are related. So, if you have written energy balance and see how material balance and energy balance are related and deal with both material and energy balance together in the design of reactors involving heat effects. These are instances there are huge chemical energy released because of the reactions or required to conduct the reaction both cases we have transfer heat through an appropriate device in the reaction equipment; so energy balance is crucial to our process.

(Refer Slide Time: 48:32)

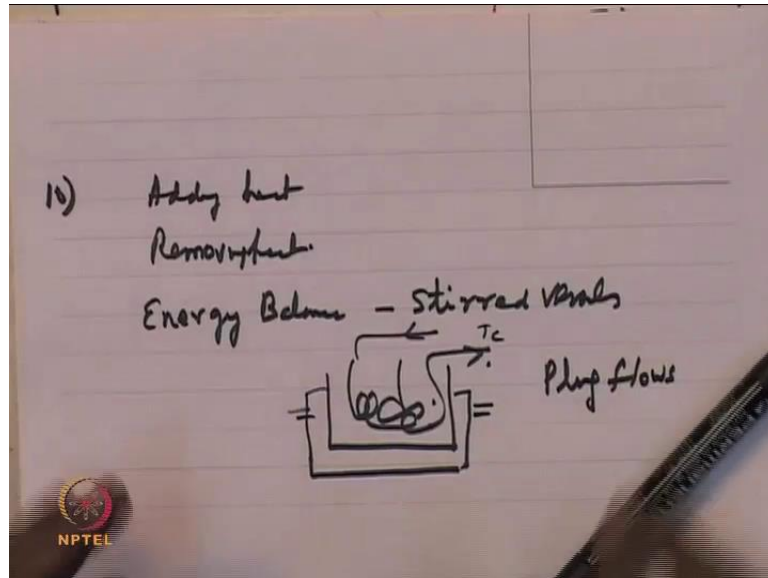


Now, energy balance can be stirred vessels; now stirred vessels we pointed out we had stirred vessel like this and we said we have a coil into which putting a cooling or heating fluid. Now, this coil instead of putting a coil put a jacket; let see that is also is good through which circulate a fluid and then take out a fluid; so there could be various ways there could be you can put energy in and energy out.

But important point is that in your equation in mathematical description you must appropriately account for energy going in. So that we energy going in which form it is going in lets typically goes in the form of enthalpy; the energy that come out may be in sensible heat and so on. So, you have to appropriately take that into account so that the very huge amount heat release appropriately; it can be removed through a device we can

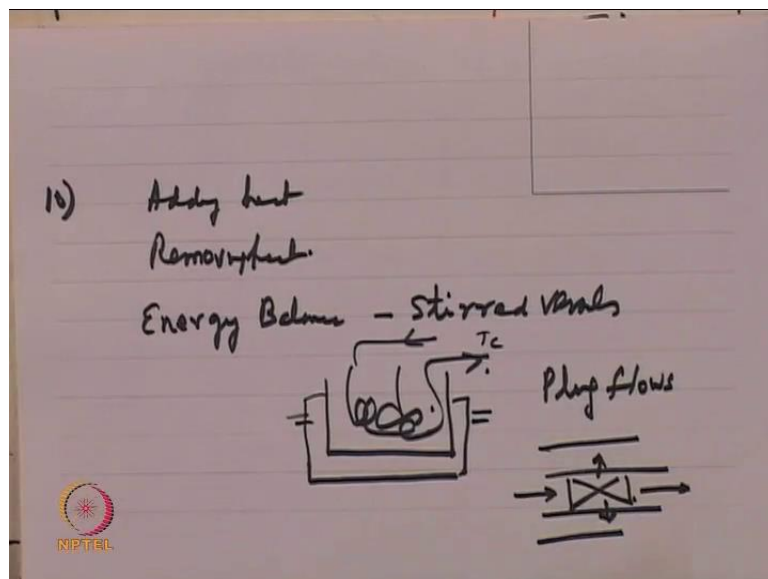
design and incorporate into the system. So, energy balance stirred vessels energy balance for plug flow vessels.

(Refer Slide Time: 49:41)



So, let us appreciate how the stirred vessels the removal of energy is relatively simple because the fact that it is stirred and therefore, heat transfer coefficient requires satisfactory; we are able to remove the heat add heat more effectively.

(Refer Slide Time: 50:04)



When it is a plug flow vessel the vessel like this; when the flow inside is gas or liquid we have to remove only through external heat exchange and here the situations are for more



involved and the designs have to be proper. More importantly, our equations must be adequately represented how these changes occur and what are the heat transfer coefficient involved and so on, which you will take into an account when we write our energy balance. We will explain more things when we go along.

Thank you.