## Chemical Reaction Engineering 1 (Homogeneous Reactors) Professor R. Krishnaiah Department of Chemical Engineering Indian Institute of Technology Madras Lecture No 10 Design of Batch Reactors Part 1

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The first 5 questions or 6 questions what we have discussed, that is the starting point for our course. Ok, what is the first question?

(Professor – student conversation starts)

Student: What is chemical engineering?

Professor: Second question?

Student: What does a chemical engineer do?

Professor: Third question?

Student: How does any chemical process start?

Professor: Yeah, fourth one? No. How does any chemical process start? That is I think third

question. Yeah fourth question was chemical reaction?

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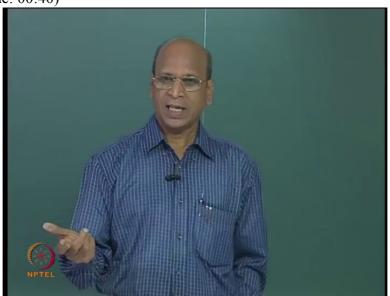
Student: What is chemical reaction engineering?

Professor: Fourth is what is chemical reaction engineering? And fifth question?

Student: What is the information necessary for reactor design?

Professor: Yeah, information required for reactor design.

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And then of course, heterogeneous, homogeneous and all that we have discussed, Ok. So we finally ended up with this diagram, again I am trying to draw this. So reactor, what is this? Input yeah, output, this one kinetics, contacting, yeah then here we have?

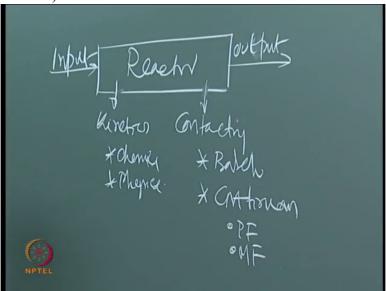
Student: Chemical, physical

Professor: Chemical

Student: Physical

Professor: Physical, here we have batch. We have continuous Oh, and here we have P F, M F, Ok. That equation I do not want to write. So please remember

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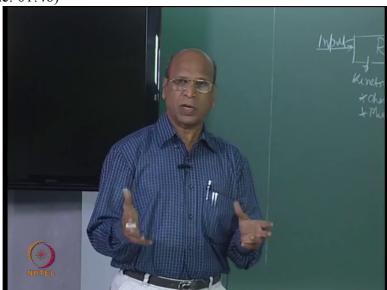


this diagram. You will have all the information that is required for reactor design, Ok. Please do not forget that.

(Professor – student conversation ends)

If anyone asks you what is the information

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required for reactor design draw this figure Ok and then explain what you, what you have to I mean, explain that is what is the meaning of physical kinetics, chemical kinetics, batch and

continuous and we have also discussed when do you choose batch and when do you choose

continuous, Ok, physical, chemical also we have discussed saying that in physical kinetics

when you say, sometimes you will be surprised also, I will derive also after some time, that

kinetic expression will not be there at all, that chemical kinetic expression will not be there at

all.

It is only the physical equation, mass transfer equation that is what what you have to

substitute in the reactor design expression. That is what is your minus r A. Your minus r A

will be simply K G into C A B minus C A S, where C A S is the concentration on the surface

and C A B is concentration on the bulk, in the bulk, Ok.

So that is why that physical kinetics will automatically come into picture. That we will do,

derive later. But when you are talking about continuous and, sorry contacting batch and

continuous when do you choose batch system? I think we discussed. I think it is better for

me...

(Professor – student conversation starts)

Student: small rates 0:02:58.9

Professor: Ok, small, small production rates, Ok. So then, that is only criteria or is there any

other criteria?

Student: Reaction is very slow.

Professor: Yeah, very, very slow reaction yes.

Student: Residence time.

Professor: It is not residence time. Residence time you can also use continuous system,

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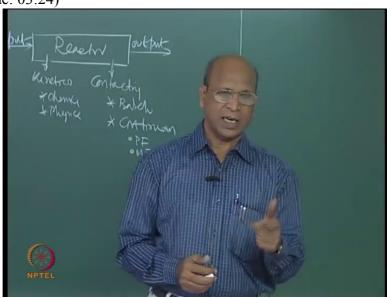
yeah so that is only criteria?

Student: When you have 0:03:20.7

Professor: What did you say the first one, batch?

Student: Batch small scale production

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Professor: Small scale and then, second one what you said is?

Student: flexible

Professor: Very slow reaction, that is all? There is another one important point.

Student: Flexible

Student: When you have unsteady

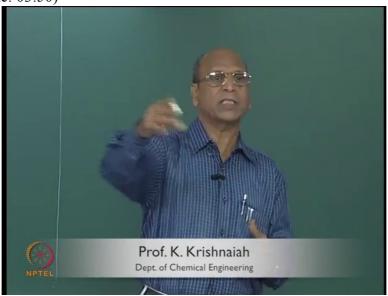
Professor: Batch reactor is always unsteady state.

Student: Unsteady state.

Student: Seasonal production

Professor: Yeah, flexibility in production. That point also is very important. When you need some flexibility with production that means you are not dealing with one product. You are dealing with maybe,

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5-6 products.

(Professor – student conversation ends)

So if you have 2-3 batch reactors, you can produce any time these 2-3 products, ok. That means there is no continuous demand for the products. So based on that you will choose which product you have to produce now. For that batch is the best system.

So but automatically that total production rate also must be small. It cannot be very, very large and still you have flexibility, right? When you have, when you want to have that kind of flexibility for very, very big size plants you have to go for only continuous, that is all. I mean there is no other choice, Ok. Good.

So that is why that important point also, please remember, three important criteria, you know many books will not give this information. Even if they give, they will simply write in one corner one sentence where you do not have, you know, you cannot go to that particular sentence and then remember it.

So that is why I am telling you these are the things, basic things that are required before we start reactor design, actual expressions because you should know what is the information required, you should know what is the meaning of chemical kinetics, physical kinetics because this will differentiate whether you will have heterogeneous reactions or homogenous reactions.

And here when you come in contacting you would like to have contacting either continuously or batch and now if you get a job in industry and you go and the people may ask you, OK, now we have a new product coming this size so you design the entire plant means you should do that. Because entire plaint design starts with only reactor design, first. Ok.

So because we have a stoichiometric equation already they would have given you and then they would also tell you production capacity or otherwise they will ask you to go for, literature, not literature what is that, market survey and from market survey you will get what is the production rate and if it is very, very large you automatically decide continuous.

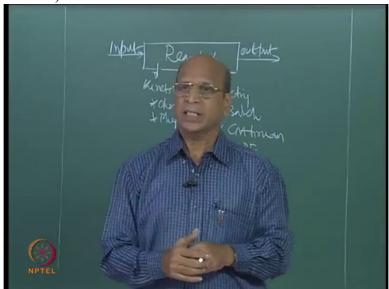
If it is small, then you know, I told you, you know may be it is 10 tons, 15 tons, 20 tons Ok, or 1 ton definitely yes but we have some,

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yeah gray,

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some gray areas where may be between 10 to 100 tons whether you go for continuous or may be batch. So for that you have to now simulate the whole system on the computer and then try to find out economically whether it is feasible to go for, yeah continuous system or batch system.

But if you have let us say 10000 tons per day if you want to produce, definitely there is no choice, no batch. You have to go for only continuous. If you are going only for 1 ton again you have to go for only batch. I think you know there is no point in designing a continuous system for that. So these are the things.

So then again we have also discussed, in continuous we have 2 choices, plug flow and mixed flow. And we discussed last class, that plug flow you will go for only very short residence times and short residence times is mainly for gas phase reactions. Because gas phase reactions are very, very fast. Even if there is catalytic gas phase reaction, the reaction time is again very, very small, seconds.

Why? Because by definition of plug flow you have to maintain very, very high Reynolds numbers, velocities, right. So when you are maintaining very high velocities, if you need very large residence times, your length of the reactor will be very, very large. You cannot have, I mean automatically diameter increasing. Because when you increase the diameter you cannot maintain plug flow, right?

Plug flow means flat velocity profile, right, one of the definitions which is also right but the correct definition is each and every particle must spend exactly same time there, yeah. So that condition will come when you have only flat velocity profile. Flat velocity profile, fluid mechanically you get only when Reynolds number equal to infinity. So that means velocity equal to infinity. If you fix this diameter.

So when velocity equal to infinity, you cannot provide you know, length by infinity. Always zero velocity. Length by velocity equal to t bar, mean residence time. So this velocity is infinity means you can provide only zero time in the reactor. That means all plug flow reactors, theoretically speaking should have zero reaction time.

Because we do not use zero reaction time we now say that if the reaction time is very, very small in minutes or seconds, then you go for only plug flow. And all packed beds are also imagined as plug flow reactors. Why? Because you can very beautifully get a flat velocity profile in packed bed reactors.

That I will discuss when we are coming again to separately designing packed bed, not packed bed, plug flow reactors, Ok, good. So now mixed flow. Mixed flow generally used for very, very, Ok another thing also for plug flow, so Ok, one is residence time, yeah. What is the another criteria?

(Professor – student conversation starts)

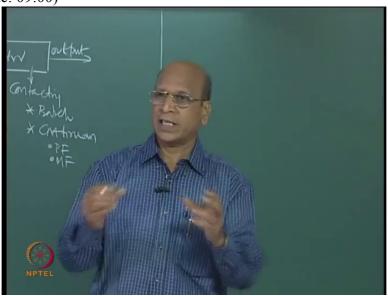
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Student: Exothermal

Professor: Exothermic reaction. Because it is impossible to maintain isothermal conditions in

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a linked reactor, Ok. It cannot. That also we will discuss when we talk about plug flow reactors again. It is not possible. There will be definitely some temperature variation. And if you want to have exactly one temperature, in a plug flow reactor you should know, you should put infinite number of heat exchangers with different capacity, Ok. That also I will explain to you. That is not possible.

(Professor – student conversation ends)

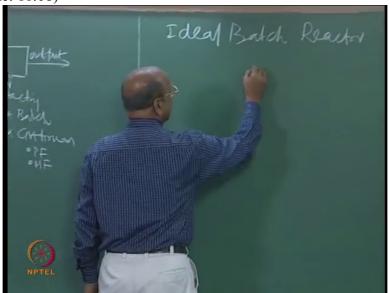
That is why if highly isothermic reactions you automatically go for mixed flow reactors. Where in due to mixing you can maintain one temperature and one concentration. That is the definition of the mixing by the 0:09:38.7. Ok. So those conditions. Now when you come to mixed flow, when you have very large residence times like liquid phase, liquid phase reactions will take place in you know, 8 hours, 10 hours, 15 hours. If it is biological waste water treatment I told you, three weeks, four weeks, one month. One month is four weeks anyway, Ok. Yeah.

So much time is required for liquid phase reactions. And many industrial reactions will be definitely between 4 to 12 hours. You know, you should have seen in the labs also, esterification reactions, esterification, saponification reaction. These reactions are 6 to 8 hours or 6 to 10 hours, Ok. So to provide10 hours mean residence time you need a tank. Because the flow rate and volume of tank will give you that much residence time.

That is the reason why you go for mixed flow system for liquid phase reactions. And another best advantage for liquid, mixed flow is that, exothermic reactions. If there are exothermic reactions, happily go for mixed flow and mixed flow is the best to control, right. So this is the criteria.

So now let us start deriving first the batch reactor. Let us take batch reactor and afterwards we will take continuous reactors. Ok. So we are now discussing about derivation of ideal batch reactor, yeah. So you know now very well that all the batch reactors,

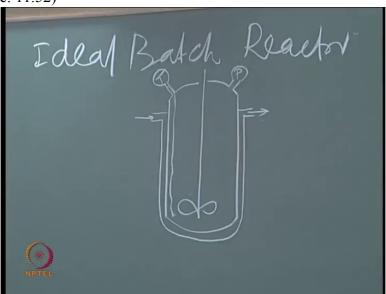
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normally in our textbooks, we will have drawn something like this.

There will be a jacket and then you will have a stirrer, this is closed and then you will have a pressure gauge. Then we will have temperature. Ok, so of course here you may have temperature measurement through thermocouple or something. Thermometers no one will put

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but thermocouple, Ok good. Yeah. This is how it looks and we will fill up normally till this point.

And when you are talking about reaction mixture, that volume, when you are deriving it actually, so that when you are calculating it, volume will be only; this is the volume, reaction

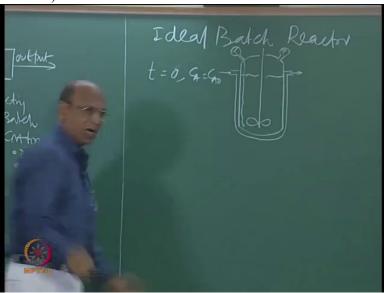
mixture. This we call it as vapor space. In case the reaction is taking place around may be 120, 150 if the vapor pressure of these reactants or mixture, reaction mixture is more then there will be some vapor forming in the top. That has to be there, Ok.

So you cannot also take it out continuously because you know, concentrations may change. So that is why you just leave it and then close everything and there may be dangerous chemicals where you may to really tightenly close. Or otherwise if it is very, very harmless chemicals, even without the top also you conduct the reaction, Ok. That means you know, this part will not be there.

It is not scientific way of doing and, but anyway that is also possible for us. So this is the one. And why do you call this as ideal batch reactor? What do you mean by ideal batch reactor? So all in these reactors we are only assuming that we have only ideal conditions, ideal contacting, Ok. And first of all, the question is why should we assume this ideal condition? And what is this ideal condition?

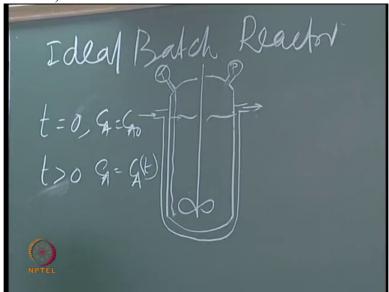
So ideal condition for batch reactor, what do you think? What are the conditions? Why it should be? But normally what we do, in the batch reactor we put the concentrations at times t equal to zero, Ok, time t equal to zero, C A may be C A naught,

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some concentration and after some time greater than zero, you will have C A equal to some concentration which is a function of type continuously decreasing

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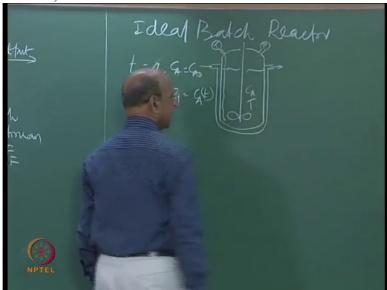


if it is a reactant or it is a product continuously increasing. That much we know.

Then we will, yeah, we will charge the reactor with whatever amount may be 1, 10 or 500 kgs whatever and then we start stirring. Normally what we do is we start the heating system if the reaction is taking place at high temperatures, may be 100 degree Centigrade. So till then even though we have the reactions there, all that we do not consider. Even though we can consider you know, definitely you know how to do that. Not much mathematics are required but still we can do that, yeah.

So then we will wait till that reaction time is complete. How do you know that the reaction time is complete? That is what what we are going to derive now for, from the equations, good? So this is what. And as someone was telling that, Ok, I have this setup and I put this and I started the stirrer and what I expect inside the reactor is, at any time inside the concentration of C A and

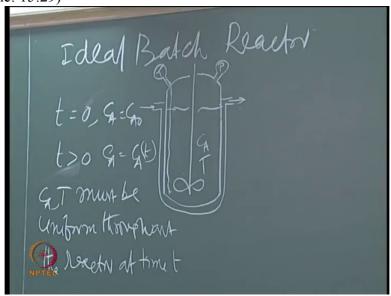
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temperature must be uniform throughout. Ok, that is the ideal condition. Ok

The ideal condition is concentration and temperature must be uniform throughout the reactor at any time t. It is only uniform. It is not same. If it is same means there is

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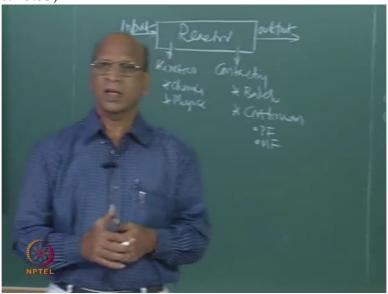


no reaction. All the time if it is same only, C A naught, then there is no reaction. Ok, it must be uniform throughout at any particular instant of time when you have looked, right? So Ok now my question is this is the condition for ideal batch reactor but why should I assume that? What will happen if I do not assume?

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(Professor – student conversation starts)

Student: Calculate the final conversion only; you have to make this assumption. Otherwise you cannot calculate that. How much of

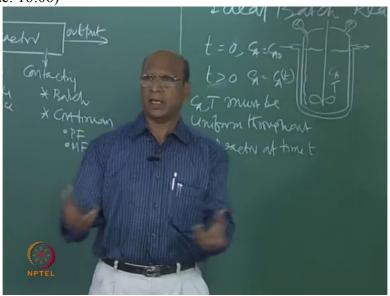
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the reactants are converted into products?

Professor: Why? I think, because I can take always sample, and then find out what is the

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concentration.

Student: Mathematically we will not be able to model.

Student: Different concentration no, every molecule has different concentration, so it is not

uniformly present in sample.

Professor: So?

Student: We cannot say at what time the reaction will be completed.

Professor: Any other ideas?

Student: 0:16:31.1 generated due to

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Professor: What are the non-linearities you are talking?

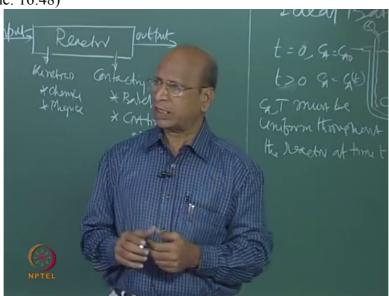
Student: Dependence of concentration

Professor: But what is the meaning of non-linearity?

Student: 0:16:44.4

Professor: That is there, already non,

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that equation is already non-linear, Redlich equation.

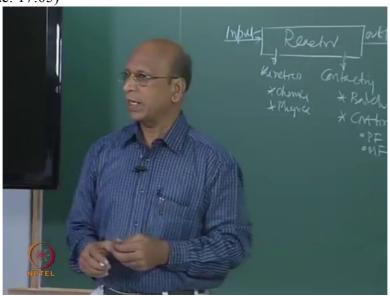
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Student: 0:17:01.2

Professor: No, how can I avoid? See, even though if I have uniform stirring,

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how can avoid non-linearity of rate expression with temperature change? Or if you have second order equation, second order rate expression, how can I assume that it will be first order? You understood linearity, no? What is meant by linearity? There are no flow rates; it is the batch system we are talking.

Student: Theoretically we are saying 90 percent conversion

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should be in time t,

Professor: Yeah

Student: Practically we are able to get only 85% of the conversion; we think that there is still a scope for increasing up to 90 percent though it is not practically possible

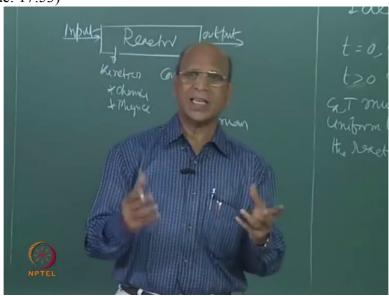
Professor: But why is it not practically possible? What are the things you have ignored

practically?

Student: There are non-idealities.

Professor: What no-idealities?

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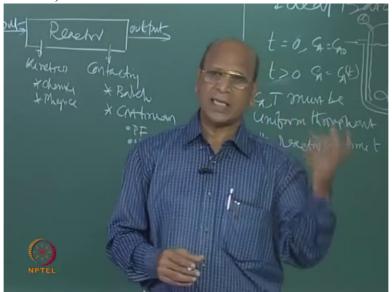
Student: There may not be proper mixing of the....

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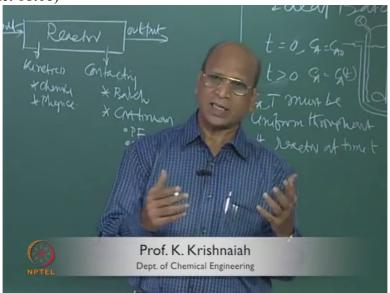
Professor: Yeah I mean what are the non-idealities? Because we have ideal batch reactor, so what kind of

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non-idealities we can expect? Only, yeah only mixing. Right. What I am asking is, if I ignore that

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where is my problem coming?

Student: Rate....

Professor: Ok, it is different. If I do not have definitely good mixing, so definitely it will be

different. So what?

Student: The conservation between the, conversion may not be...

Professor: Yeah, that is very important. The rate expression which we are getting, I do not

know how to write. The rate expression is a function of

Student: Temperature

Student: Concentration

Professor: Temperature and?

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Student: Concentration.

Professor: And concentration. Forget about temperature now, right now. We only talk about concentration. You have non-ideality. That means it is not uniform mixing.

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So it is function of concentration. Next concentration is which concentration? The concentration here, or here or here or here? Where? Yeah.

(Professor – student conversation ends)

But you know, definitely my problem will solve if I am able to have throughout only one concentration. Then I know definitely my rate is a function of that concentration. Otherwise if the concentration is changing at various places, now I should get, I should measure at each and every point, I should get some average of that, weighted average for example in this volume, I take 1 percent volume what is the concentration? I take 5 percent volume, what is the concentration? Another 1 percent here, what is the concentration? Another 10 percent here what is the concentration.

I have to sum up all that and then take some average, some volume average which is headache for me. Why? Because fluid mechanics already taught me better design a, how to design a stirrer, so you do very efficient stirrer so naturally you will avoid all that measurements, here, here, here, here, here, here, here, here is first of all, how do you measure?

You have to put infinite number of probes there. Ok, if you are directly reading. Otherwise like you know, how you took the sample using pipette. How many pipettes you have to use? What length? And that fellow is stirring inside. That may break, you know the pipettes. All this, why that problem?

Simple problem is design a good stirrer, mixer, your problem is solved. So that is the beauty in assuming that we have ideal batch reactor, ideal mixing. Ok. Now you know no, because most of the time we will not discuss this part. We will say that, assume uniform mixing. That is all we will say. So that will give you uniform concentration and uniform concentration. But we never ask so what?

If I do not assume, what will happen? What will happen is your life will be miserable in measuring, in at every point. And after that you have to average it out. Ok. So some kind of weighted average or you know, either weights you have to use, volumes you have to use, all that. And first of all, how do you measure them throughout the reactor?

And in the lab it is Ok, maximum I may take 1 liter, 2 liter, 5 liters. But industry it will be 5 meters cube, one well, big well. So that well, I think inside that you are stirring and all that, how do you take the samples there in the well? So to avoid that we will say that yes, now I can design a perfect stirrer and that is much easier for me than measuring the concentrations at various points.

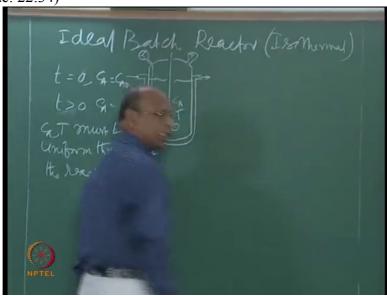
Now let me assume that I have a perfect stirrer where it gives me uniform concentration and uniform temperature. So that is the meaning of this assumption and if that assumption is not there, then you have a problem to define even what is rate. Because rate is the function of concentration and temperature.

Temperature is varying at various places. Concentration is varying at various places. Which rate you are talking? So when I am writing my material balance, I do not know which rate I have to write. Unless you take again some average rate, right? So that average rate is given by your stirrer that is all. What we are doing is instead of you doing all that, you are asking the stirrer to do that that is all.

When it is perfectly mixing, the contents will be only with one concentration and one temperature so that you can happily measure that concentration, only one concentration you have to measure, one measure and then you can write the rate expression. So once we know that, then how do we write the expression?

Like the material balance, first I think first we are doing only first, isothermal. Let me also write here,

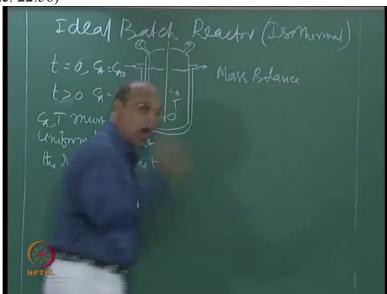
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and non-isothermal we will do it after you learnt something from isothermal reactors that we will do later. So here and you know we have one universal material balance equation, it is a mass balance equation what I am telling. I am not writing energy balance. Energy balance I will write later.

So mass balance equation, always when you are writing mass balance equation please remember

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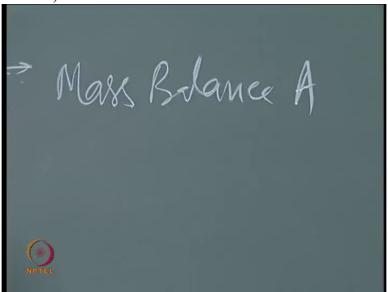
you have to specify you are writing for which species? Mass balance is always for individual species where as energy balance is for whole thing. You do not have to differentiate, Ok. That is the beauty in you know, heat transfer because it simplifies.

Whereas mass transfer every species you have to write. And always in our course, our species is A, reactant A which is the limited reactant, you know what is that, limiting reactant, which is a limiting reactant or key reactant that is also another name what we say, right? So that means that is the one which is really governing the rate.

You heard of definitely what is pseudo homogenous, yeah pseudo first order for example. Actually that is a second order reaction, A plus B going to some reaction, then I am taking may be 100 or 200 moles of B, and only one mole of A. This is what we call pseudo-homogenous first order reaction with respect to A, why A?

Because I can see only the concentration change with respect to A. With respect to B I cannot see because I have 500 moles or 200 moles. Practically there is no concentration change in that, Ok. So that is why we have to write only for a particular species and here we do for key reactant and all the time when we write mass balance A that means that is our key reactant,

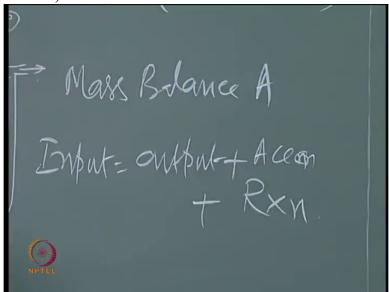
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our limiting reactant. Ok.

The universal equation always what we have is input equal to output plus accumulation, yeah R x n, reaction

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Ok, where except the problems as I told you, all other things are only written with his hands including graphs. It is worth seeing. I have a copy. I think I will show it to you once. I have a copy.

It is a library copy only. Because it is with me, it is not lost. So otherwise I think that also could have gone I do not know. It is beautiful, his handwriting. Some of his papers also, I will

also send some of his papers where he has drawn diagrams and graphs with his own handwriting and the matter is of course typed. So that is why all excellent engineers will have very good handwriting.

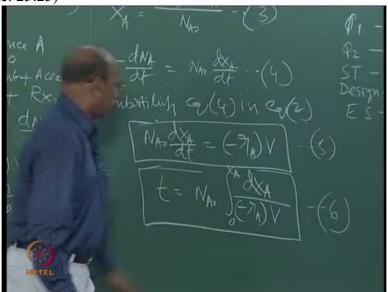
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Good.

So this is the equation what we have.

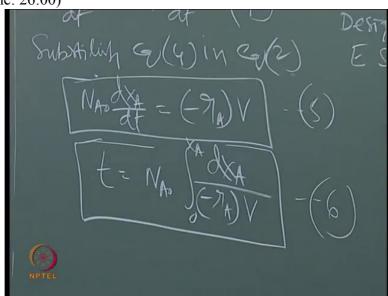
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So now this equation I can simplify if we say that, for constant density system, Ok, then this will become N A naught by yeah v equal to C A naught. Where is the, yeah. For constant

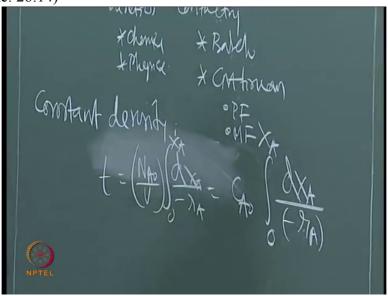
density system, for constant density, t equal to yeah N A naught because for others sake I will just write here, into d x A, oh

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integral d x A by minus R A zero to X A which is nothing but C A naught minus R A, that is the one,

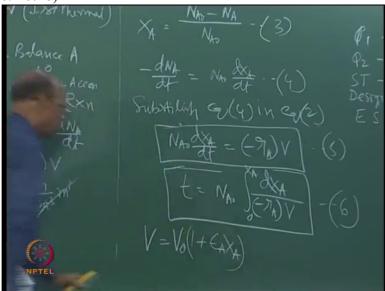
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Good.

And if the other example what I gave, volume is changing Ok, that means 1 mole giving 4 moles or may be 4 moles giving 1 mole that is volume reduction. Ok, so the volume reduction is given by Levenspiel as, yeah, for isothermal system, I am writing isothermal system, V equal to V naught into,

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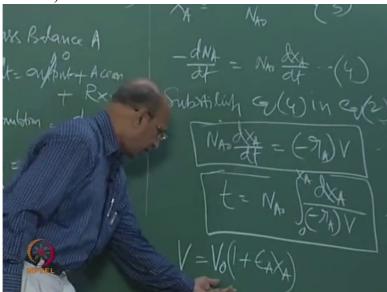
where epsilon A equal to...

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So this is the equation, linear equation what he has

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used where epsilon A is number of moles initially present minus

(Professor – student conversation starts)

Student: Final minus initial

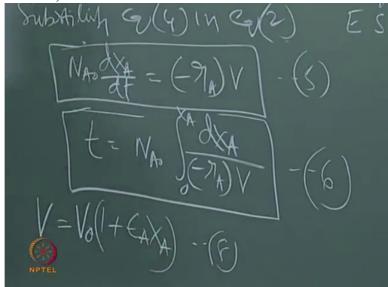
Professor: Yeah final minus initial divided by initial, Ok or volume, volume at t equal to zero, volume at any time divided by volume at t equal to zero, Ok, that equation also, what is the origin and all that I will derive. I do not ask you to blindly accept that. But Levenspiel directly says that assume the variation in volume is linear.

(Professor – student conversation ends)

Ok, so why we should assume or why we cannot assume, we will derive. I will derive and then I will let you know. Ok so that we will do after completing then contacting pattern. So then for variable volume, you will have equation t equal to N A naught, zero to X A naught. Yeah, so then d X A by minus R A, into V naught, 1 plus epsilon A X A, Ok.

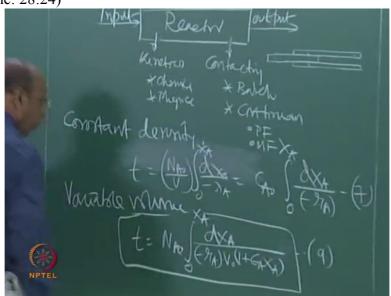
So this equation I have written no, later, after that then this is equation number 8,

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this will be equation number 9, this is the general expression again

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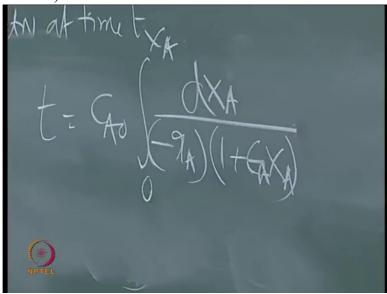
for variable volume and you know that this v naught is a constant. Yeah, that becomes A naught, good.

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So for constant density systems, this if I take here, t equal to C A naught zero to X A d X A minus R A 1 plus epsilon A X A,

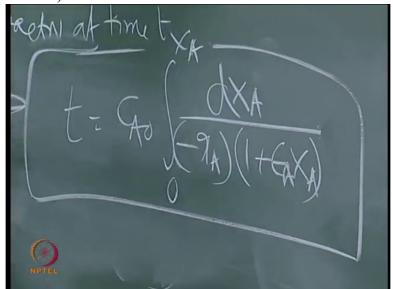
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very good, Ok, good.

So this is the equation for constant density system,

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sorry variable volume system, Ok, good. So now this equation he just leaves it without integrating, then, of course as special cases you can always do that, Ok and he also puts these in form of graphs. We are only simply putting this equation in form of graphs, this integral in fact. How do I plot this integral as a graph to get that area under the curve? Where is this? Yeah. Ok, this d X A is, X A must be in y axis or x axis?

(Professor – student conversation starts)

Student:

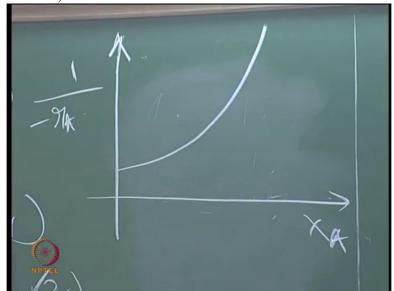
Professor: Yeah because with respect to this we are integrating that,

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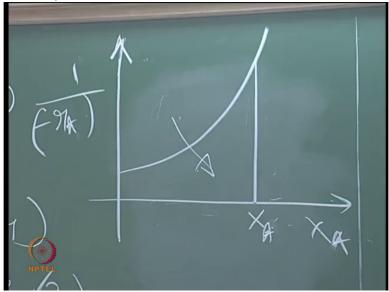
so this is X A and yeah, minus 1 by R A, Ok, so what we get here is this kind of thing,

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Ok. And yeah, actually when you plot X A versus 1 by minus R A you get like this, right? So you take till whatever conversion you want, X A and this area under the curve,

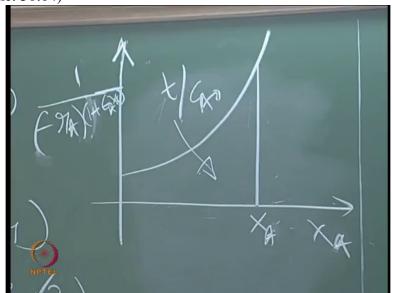
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it should have brought this one, t by C A naught this side, so in fact I should not, here also I have to add here in this case, 1 plus epsilon A, that entire thing I am plotting, Ok. (Professor – student conversation ends)

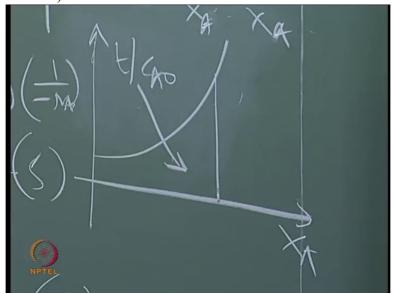
Yeah, so this will give me directly t by C A naught, Ok. So but I, if I plot this one, constant density system I have to plot this one as,

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this is variable volume right? This is variable, variable volume for constant thing, you have 1 by minus R A plus X A again giving me like this, this is t by C A.

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So that is how, because he uses, these are, even though earlier people have used, these plots are called Levenspiel plots, minus R A but I think originally also people used it but somehow I think people call this one as Levenspiel plots and idea here is, because he is an excellent engineer, Ok, I told you no. So the reason is that this equation how complicated it would be, we do not know. Ok.

So if it is a simple one we have a mathematical expression, analytical expression. But in industry, when you go for complicated reactions, I do not have to really integrate that using

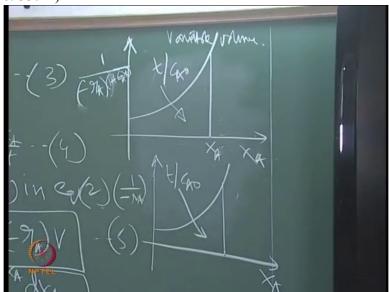
mathematics. Sometimes it is not possible to integrate. So you have to go either numerical integration or you have to go for graphical integration.

Graphical integration is this. So he will simply calculate X versus all this, different X, because epsilon A you will calculate, you will know that. And then X and then minus R A because minus R A is nothing but some equation, in terms of K C A for example, first order equation if you take. So that C A again will have C A naught into 1 minus X A but he is variable volume, that also will have, 1 minus epsilon A X A cancels and all that, but anyway, so that you will have this function as only X and, only X, that is all, nothing else. Other things are constant. Ok.

So then we can plot and get the value. Ok. That is not difficult at all. But these are the basic reactors which you also use in your waste water treatment, Ok. And of course, chemistry people also have to learn this, because the catalysts, so that is why these are the basic equations, even biochemical, they use only this equation. This minus R A will be for them either Monod's equation or Michaelis-Menten equation, Ok.

So even the other two reactions, same thing, Ok. Good. So that is why these graphical procedures must be very easy for us and I love graphs, really. Because I will tell you later you know, optimization only using graphs,

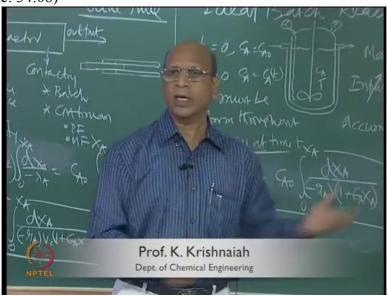
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again Levenspiel method, wonderful techniques he has developed. Simply drawing graphs. No mathematics required for optimization, Ok. Using graphs how do you optimize, that means minimum volume for maximum conversion or minimum, maximum conversion for minimum volume or given volume, Ok that also we will discuss later.

There are many exciting things to learn. Even though you have learnt once, because it will be more exciting now

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learning the same thing. Ok, good. Anyway I am thankful for you because you have forgotten everything. So that is why all these things you may appreciate. Ok, good. So I think here we will stop.

This is what is the batch reactor but surprisingly you notice that there is no volume present anywhere. These are final expressions. This is 9, this is 10. This is one final expression and this is another final expression, Ok, C A naught, right. Where is the volume coming there? And the next class we will see where the volume comes. Because finally you have to tell so much volume of the batch reactor, but any quantity you take you will only get time.