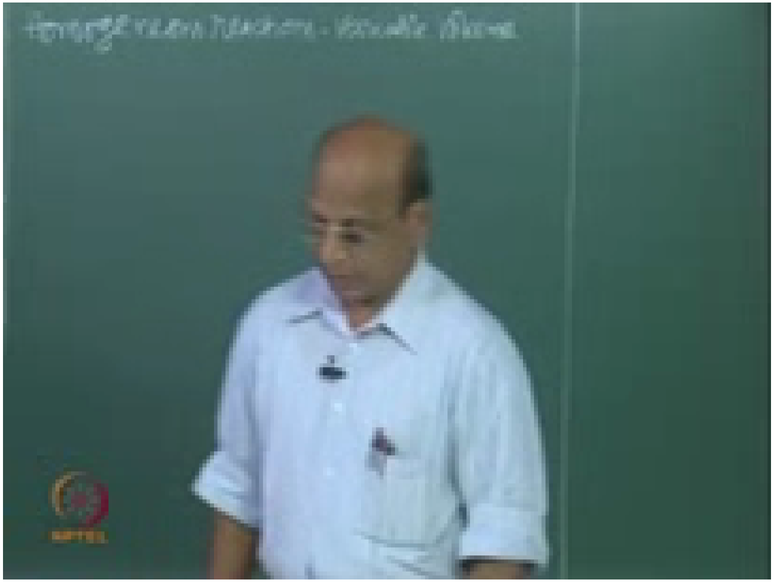
Chemical Reaction Engineering 1 (Homogeneous Reactors)
Professor R. Krishnaiah
Department of Chemical Engineering
Indian Institute of Technology Madras
Lecture No 25
Contd. and later Reaction Design of PFR

(Refer Slide Time: 00:10)



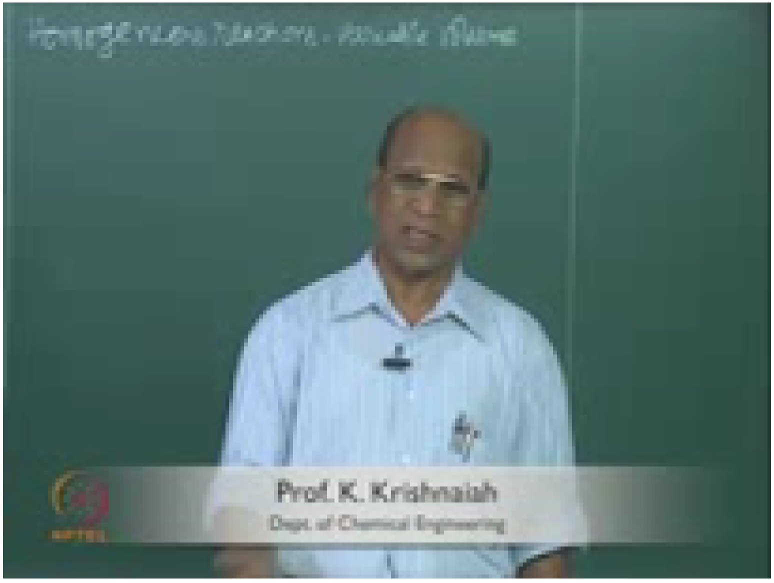
Yeah this variable volume what we have been discussing yesterday and you know for constant densities how do you write concentration, definition. How do you write concentration definition for variable, I mean for constant density system?

(Professor – student conversation starts)

Student: C A equal to C A zero by 1 minus X A

Professor: Actually what is the definition

(Refer Slide Time: 00:27)



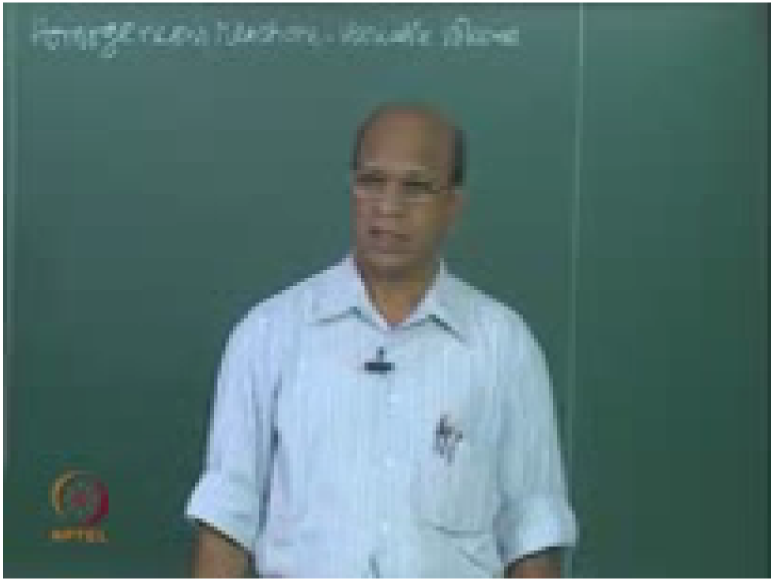
of C A, moles per?

Student: Unit volume

(Refer Slide Time: 00:30)

Professor: Moles per unit volume. So what you write is C A equal to N A by

(Refer Slide Time: 00:33)

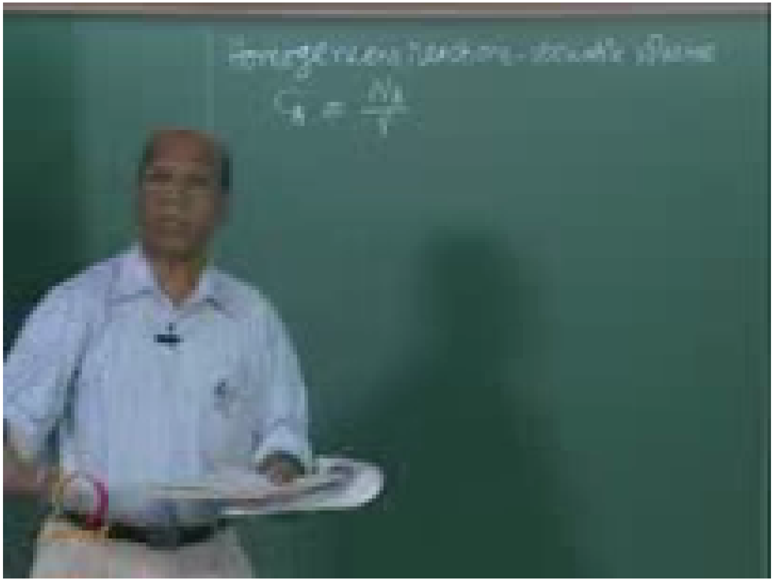


V, that V is constant so that is why straightaway you can take it as C A.

(Professor – student conversation ends)

So but when you have variable volume, even the concentration definitions also will change. Ok, so that is why we have to write now C A equal to N A by V and when I express this in terms of

(Refer Slide Time: 00:55)



conversions and this V is V naught , yeah V naught into 1 plus epsilon A X A and what are the assumptions in that? There are assumptions in that. It is truly valid for

(Professor – student conversation starts)

Student: Variable volume

Professor: Variable volume is Ok but I think still it is valid for

Student: Pressure also...

Professor: Yeah, ideal gas constant temperature

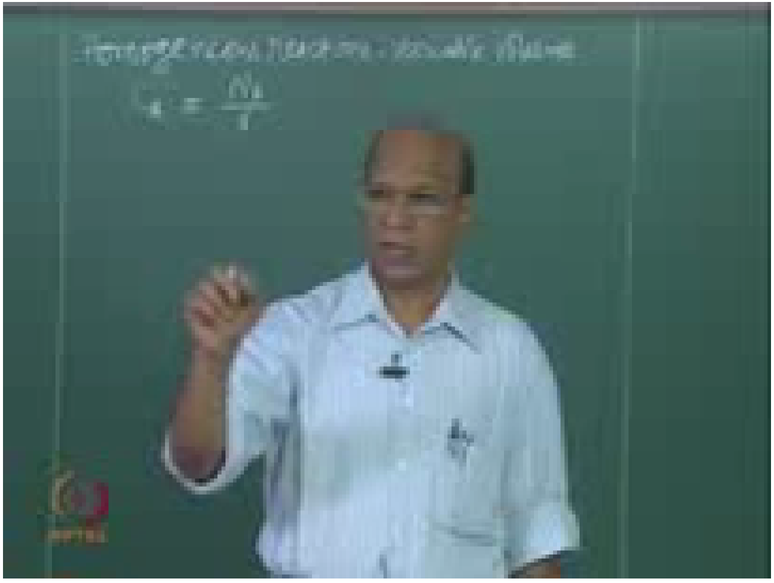
(Refer Slide Time: 01:20)

and constant

Student: Pressure

Professor: Yeah, constant pressure. So that P by P naught equal to 1,

(Refer Slide Time: 01:28)



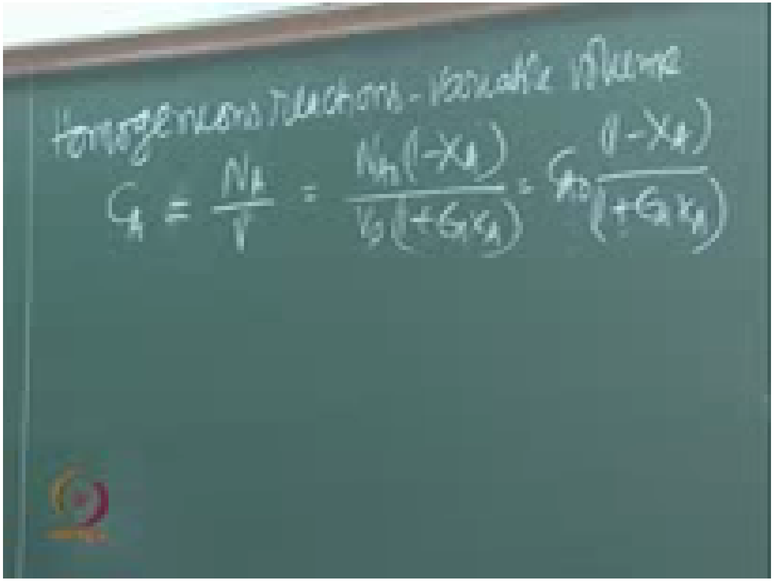
and the variable, I mean what is the other one he said, T by T naught that is isothermal system and also ideal gas.

(Professor – student conversation ends)

So please remember that, these are the things. Assumptions are very important there. So now this is the definition what we write and I have to now substitute if I want to write this one in terms of conversions, so this will be N A naught into 1 minus X A by V naught 1 plus epsilon A X A so normally this will be again C A naught. C A naught into 1 minus X A by 1 plus epsilon A X A, you see now the problem.

Because

(Refer Slide Time: 02:07)



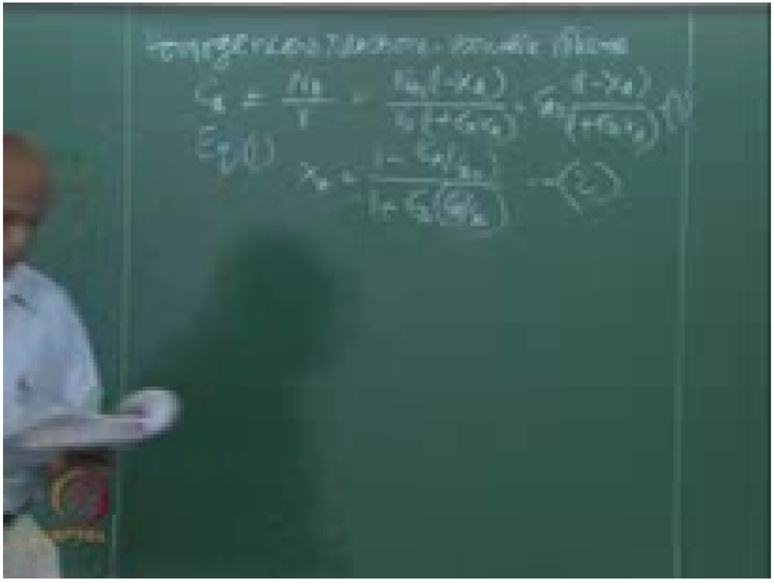
Homogeneous reactions - variable volume

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X_A)}{V_0(1+\varepsilon_A X_A)} = C_{A0}\frac{(1-X_A)}{(1+\varepsilon_A X_A)}$$

this definitely increases, you know the algebraic difficulties; you know when you are actually solving. So this is equation 1, and of course you can also get, from equation 1, you can also write X A in terms of C A. Same equation. I will simply solve for X A.

So when I will solve that I will get minus 1 by, 1 minus C A by C A naught divided by, yeah 1 plus epsilon A C A by C A naught. This is equation 2. These equations will be

(Refer Slide Time: 02:48)



Homogeneous reactions - variable volume

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X_A)}{V_0(1+\varepsilon_A X_A)} = C_{A0}\frac{(1-X_A)}{(1+\varepsilon_A X_A)} \quad (1)$$

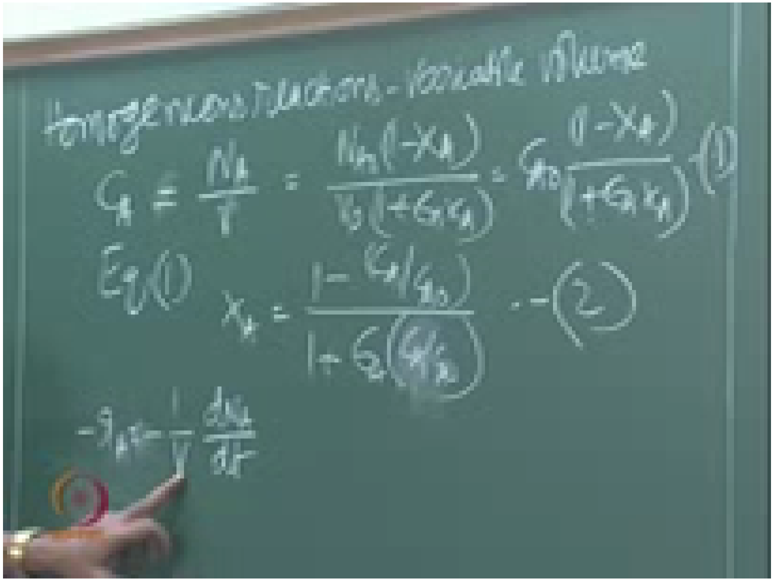
Eq(1)

$$X_A = \frac{1 - C_A/C_{A0}}{1+\varepsilon_A(C_A/C_{A0})} \quad --(2)$$

helpful to you. And even rate definition also changes. Rate is simply, Ok minus r A equal to minus 1 by V d N A by d t. This is the basic definition.

Ok but this V is also changing,

(Refer Slide Time: 03:08)



Homogeneous reactions - variable volume

$$C_A = \frac{N_A}{V} = \frac{N_{A0}(1-X_A)}{V_0(1+\varepsilon_A X_A)} = C_{A0}\frac{(1-X_A)}{(1+\varepsilon_A X_A)} \quad (1)$$

Eq(1)

$$X_A = \frac{1 - C_A/C_{A0}}{1+\varepsilon_A(C_A/C_{A0})} \quad --(2)$$

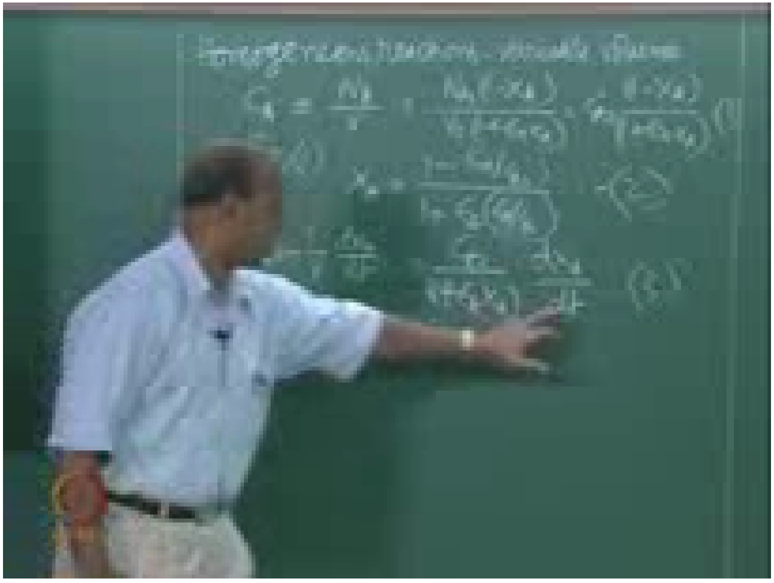
$$-r_A = -\frac{1}{V}\frac{dN_A}{dt}$$

right? So if I substitute V equal to V naught into 1 plus epsilon X A, and also if I write for d N A, because conversion definition is always moles initially entered minus moles at any time divided by initial mole. So that I think you remember. That is why I am not writing that, moles wise.

But C A definition is wrong again. You cannot use C A in terms of you know C A for X A all the time. We also write X A equal to C A naught minus C A by C A naught, which is not correct all the time. It is only strictly valid for, constant volume, Ok constant density system.

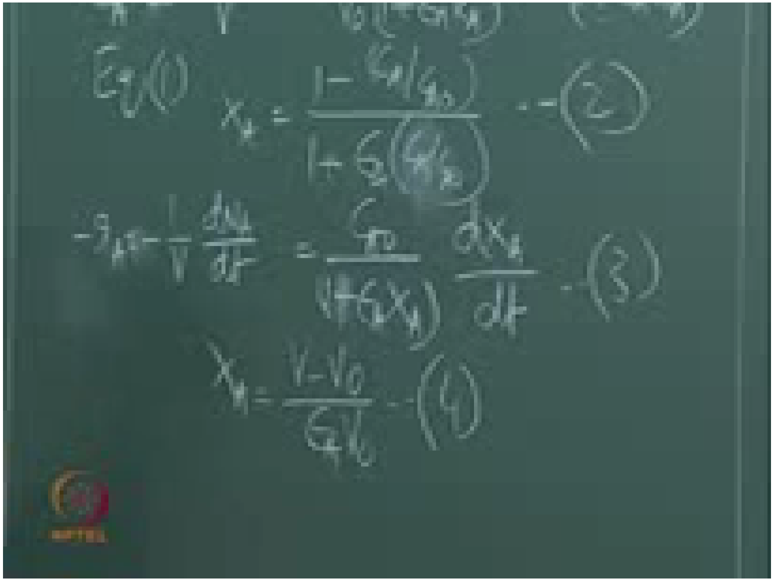
This can be written as C A naught 1 plus epsilon A X A into d X A by d T, this is, actually this is the definition of now rate

(Refer Slide Time: 04:06)



for variable volume, Ok. So now of course yeah, d X A also we know what we have written there and all that. So X A in terms of volumes, this definition. How do you get this? This is strictly for isothermal and you know ideal, ideal gases

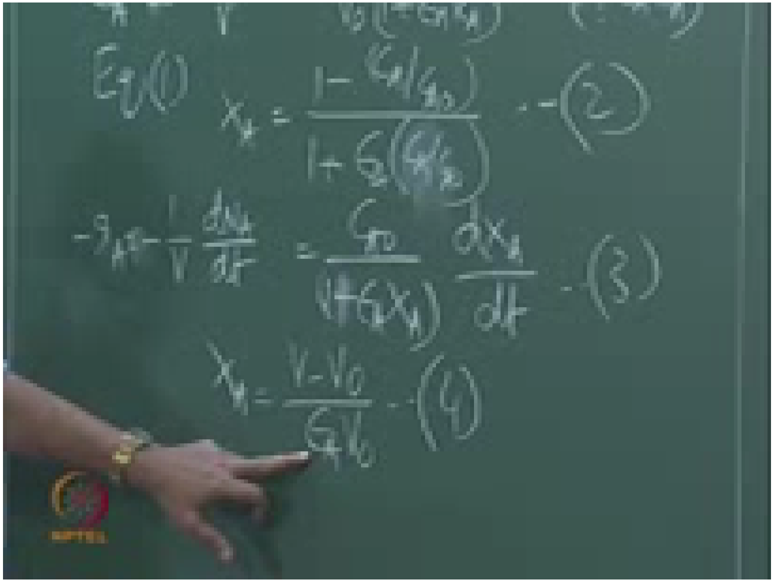
(Refer Slide Time: 04:35)



yeah and also constant pressure, sorry vari/variable, constant pressure.

Yeah, this you know how do we get?

(Refer Slide Time: 04:41)



(Professor – student conversation starts)

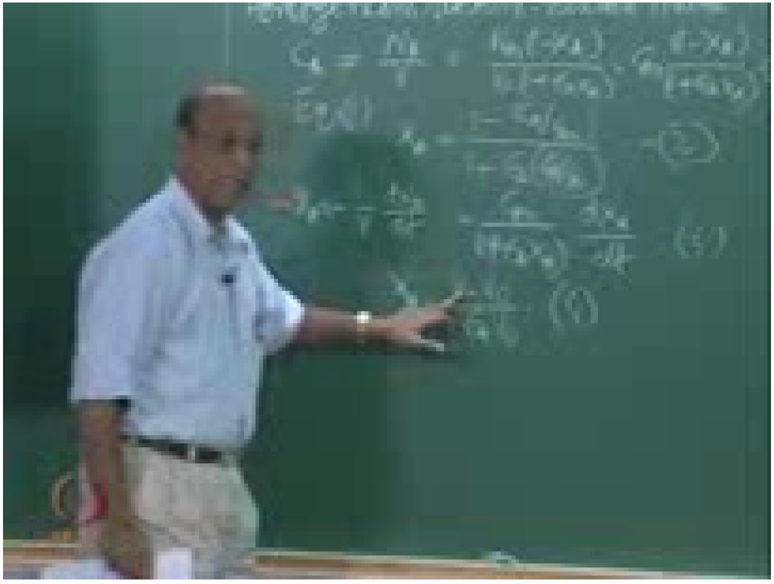
Student: V zero...

Professor: From V equal to V naught into that one Ok. This is good.

(Professor – student conversation ends)

Why I am writing all this is that you are trying to use this technique of measuring the volume and trying to find out the kinetics. Measuring the volume. This is the total volume. So

(Refer Slide Time: 04:59)



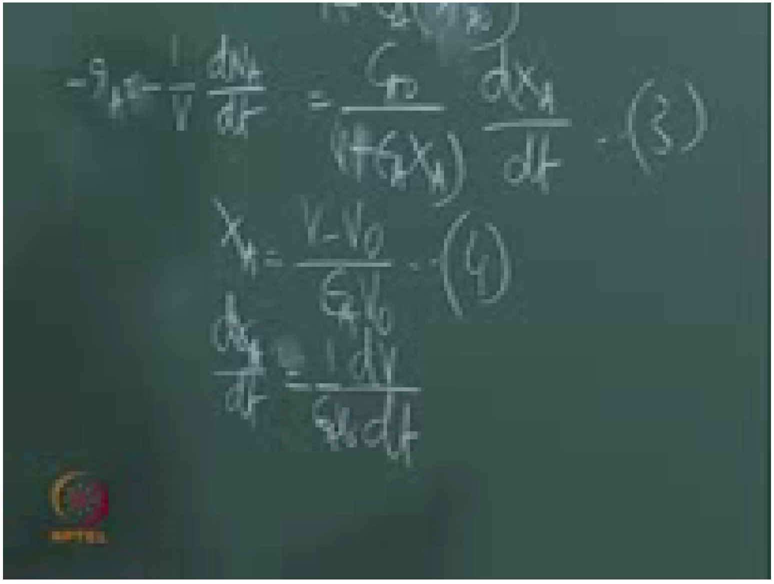
at any time t, the volume expands, right? So that volume if you are able to measure, now can you get the kinetics? Ok.

So again you can use here either integral method or differential method. So integral method when you are using, so there is another thing also which I have to tell you here, yeah, so Ok, what is d X A here, or Ok d X A by d T...

(Professor – student conversation starts)
Student: d V by d T, 1 by
Professor: Ok, d V by
Student: d T
Student: 1 by epsilon A V zero
Professor: Epsilon A V naught, right?
(Professor – student conversation ends)

So for this, yeah d X A by d T we can substitute this equation, Ok, in terms of volumes, right,

(Refer Slide Time: 05:52)



$$-r_A = -\frac{1}{V}\frac{dN_A}{dt} = \frac{C_{A0}}{(1+\epsilon_A X_A)}\frac{dX_A}{dt} \quad (3)$$

$$X_A = \frac{V-V_0}{\epsilon_A V_0} \quad (4)$$

$$\frac{dX_A}{dt} = \frac{1}{\epsilon_A V_0}\frac{dV}{dt}$$

yeah, you can substitute that equation, yeah, Ok, good, so now I will just give you with all the, this is also equation 5, I will just now try to give you for zero order reaction how do you find out volume change. That is the simplest one.

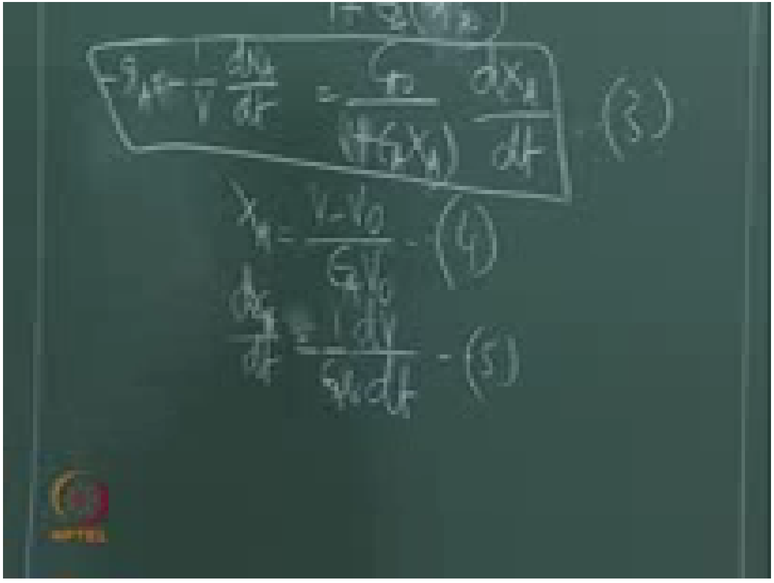
See, our idea, why I am writing all this is that, you are measuring, our idea of finding out kinetics is, either you can change the pressure for a constant volume, right, so you will get total pressure change. That total pressure you are able to convert to partial pressure, yesterday's last equation was that.

So once you know partial pressure of A and partial pressure of B, what you assume is that whether first order, or second order, integrate, and you have all that information now. So similarly when I have constant pressure and variable volume, right so there you are measuring pressure change, total pressure change.

You cannot measure individual component change, P A, P B, P C you cannot change, Ok. So that is why total pressure. Even here it is total volume what you are measuring. Once you measure the total volume, how do you now convert that into rate equation?

So this is the definition of rate now, minus r A,

(Refer Slide Time: 07:08)



$$\boxed{-r_A = -\frac{1}{V}\frac{dN_A}{dt} = \frac{C_{A0}}{(1+\varepsilon_A X_A)}\frac{dX_A}{dt}} - (3)$$

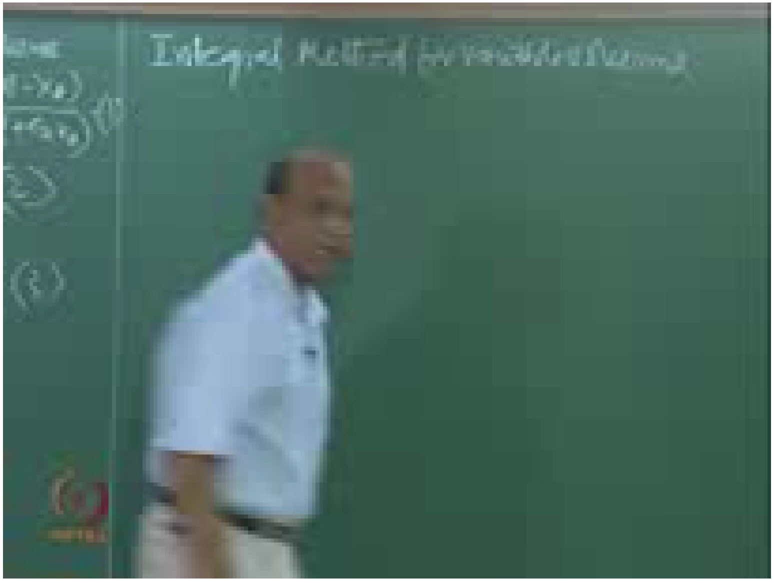
$$X_A = \frac{V - V_0}{\varepsilon_A V_0} - (4)$$

$$\frac{dX_A}{dt} = \frac{1}{\varepsilon_A V_0}\frac{dV}{dt} - (5)$$

right. So if I have a zero order reaction, Ok what is minus r A? k. So this must be equal to k, right or for zero order reaction, integral method, integral method for variable volume.

I think

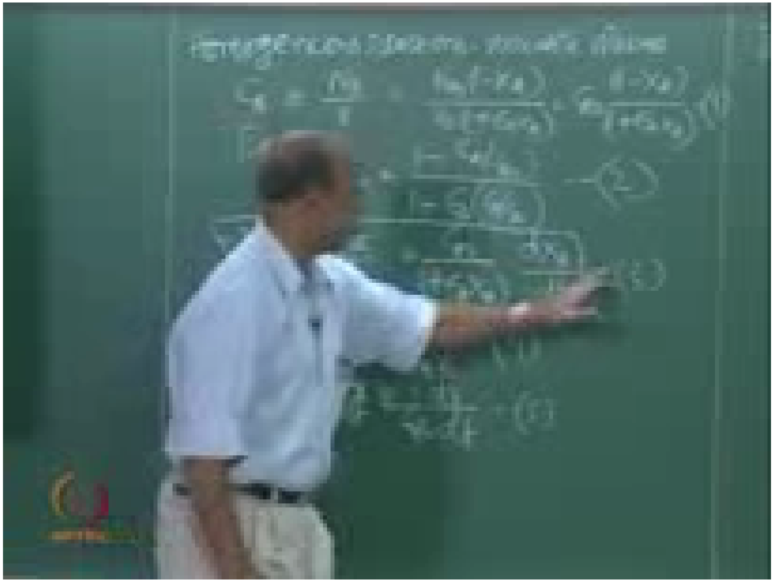
(Refer Slide Time: 07:36)



very nice problems are given in Levenspiel, very beautiful problems I think, you know last few problems of third chapter, very, very nice problems of you know, in terms of volume change, yeah. So our idea is to find out through variable volume what is the kinetics. For that we should have an integral expression if I am using integral method, Ok.

So if I am not using integral method then differential equation, that is the, yeah this equation I have to use and this is

(Refer Slide Time: 08:03)



equal to k into C A to the power of N, where N again, you know N is Ok but C A again written in terms of, yeah, C A is nothing but C A naught into 1 minus X A by, yeah

(Professor – student conversation starts)

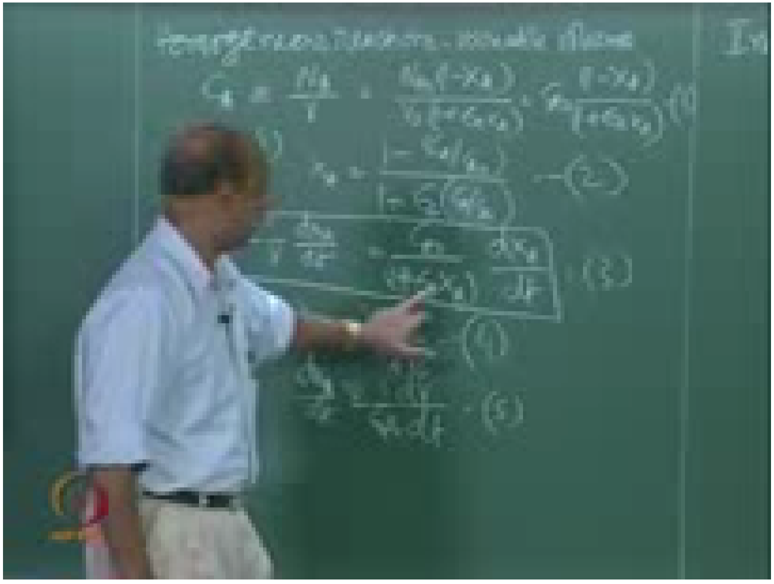
Student: 0:08:18.4

Professor: Yeah, this is where you make the mistakes. Ok. So that is why you have to do that.

(Professor – student conversation ends)

So then you can plot as far as possible in terms of straight lines, whatever information you know there, epsilon will be knowing there,

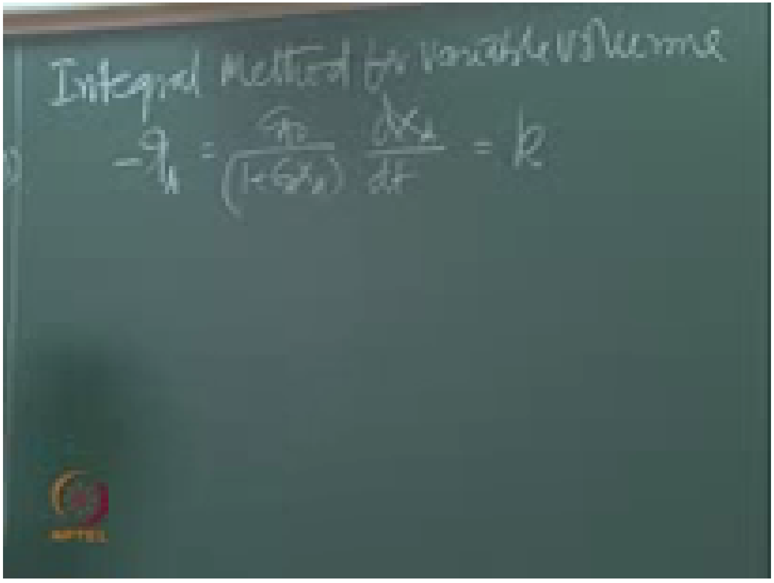
(Refer Slide Time: 08:29)



X A you are measuring there. So C A naught initially you know. And with time you are trying to find out what is the conversion, so you can do that, right.

So similarly here, for integral method, for zero order reaction, minus r A equal to, this one C A naught 1 plus epsilon A X A, d X A by d T equal to k. This is for zero order equation, right? I think as an exercise, can you convert this X A

(Refer Slide Time: 09:11)



Integral Method for Variable Volume

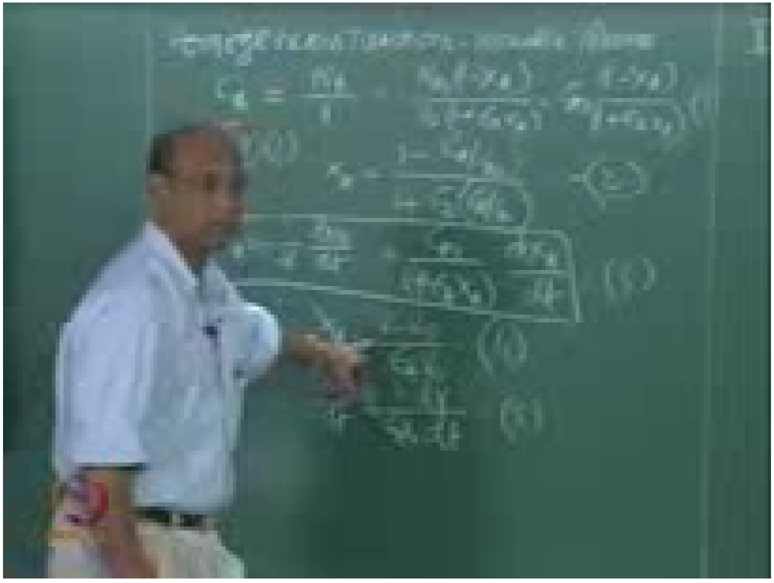
$$-r_A = \frac{C_{A0}}{(1+\varepsilon_A X_A)}\frac{dX_A}{dt} = k$$

in terms of V and then try to find out what is the volume change? I think you have here, what is d X A by d T. Can you tell me the equation?

Because this is I think the simplest one which I can give you without losing much time. If I give slightly complicated equation you will have more problems. What I am asking you is, forget about this one. These two you have to take. So this is 5, this is 6. Now get me an equation in terms of volume. V by V naught, V by V naught equal to, what 0:09:42.8, not able to get? Not able to get.

(Professor – student conversation starts)
Student: 1 by V naught into 1 plus
Professor: Tell me, straightaway this is only
Student: 0:09:54.4
Professor: For X A you have the equation here, no?

(Refer Slide Time: 09:56)



Yeah, so d X A by d T you substitute and then try to integrate. What do you get?

(Refer Slide Time: 10:05)

Student: V is equal to V naught e power of K epsilon C A by C A naught.

Professor: Can you tell in terms of log V by V naught?

Student: l n of V by V naught is equal to k epsilon A C A by C A naught.

Professor: Yeah let us see. Some more. Let us see some more people.

Student: (discussing)

Professor: k epsilon

(Refer Slide Time: 10:42)

Student: epsilon A K T by C A naught.

Professor: Very good, very good but all

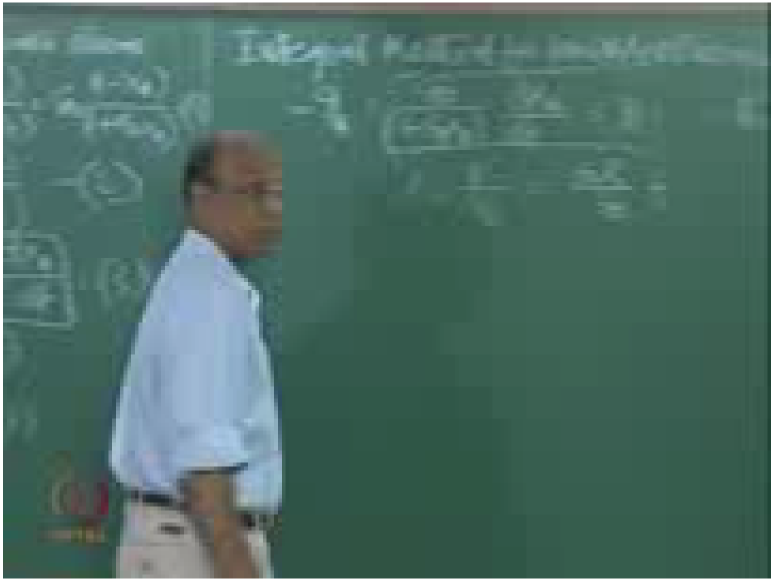
(Refer Slide Time: 10:45)

of you should do this. All of you should do this. I think I do not want to, yeah those who have not done, definitely I think they have to practice more, right, they have to practice more.

(Professor – student conversation ends)

So what you get here is l n V by V naught equal to epsilon by, yeah C A naught into T.

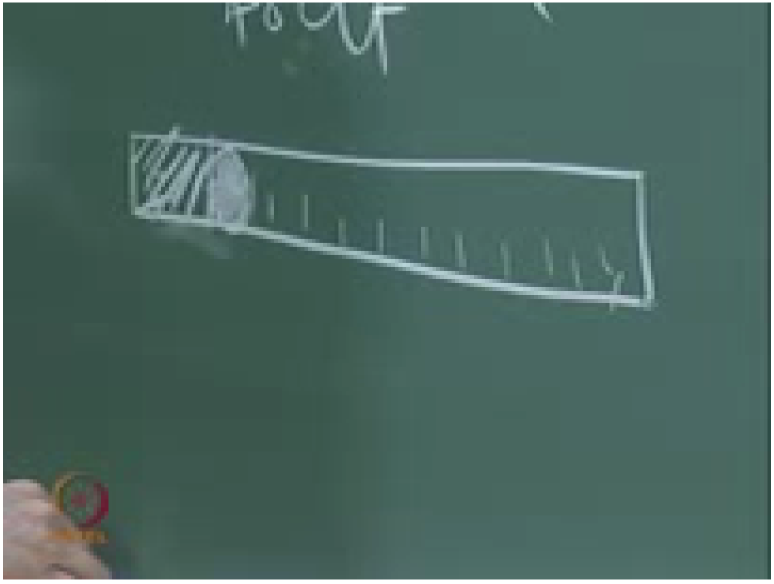
(Refer Slide Time: 11:16)



So this is the equation after integration. Ok, so now you know I am using an integral method. So what is the thing? So I have now, I do not measure X directly now. Because that is the idea.

Because how I take is, Levenspiel method is that is you know, I mean he has used wonderful techniques here. He just takes a tube where he fills up somewhere here the gas, batch system, Ok that is V naught for us, then he will put a graduated scale and then he puts a small ball here. Ok.

(Refer Slide Time: 12:05)



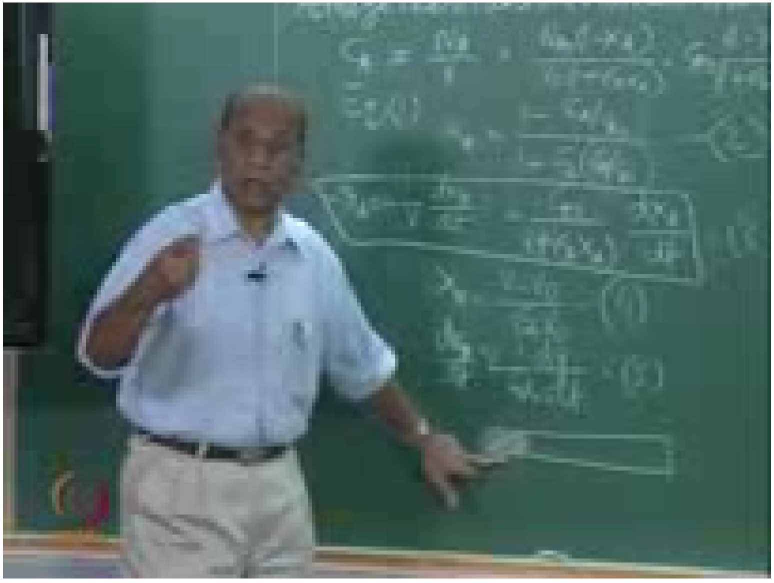
Otherwise I will put the color, yeah.

You would have seen rotameter no? There are some rotameters for very low flow rates that ball as spherical. It need not be, you know that cone shaped. Cone shaped and all that will give more stability but this is a bad design but still at very low flow rates, this sphere is, it can be used.

So similarly here, this will, this can easily float, this can easily move the moment reaction started. Let us say this is the reaction, actually this is a reactor for you, batch reactor. So this entire reactor you put in hot water. Let us say the reaction is occurring around 80 degree Centigrade, right.

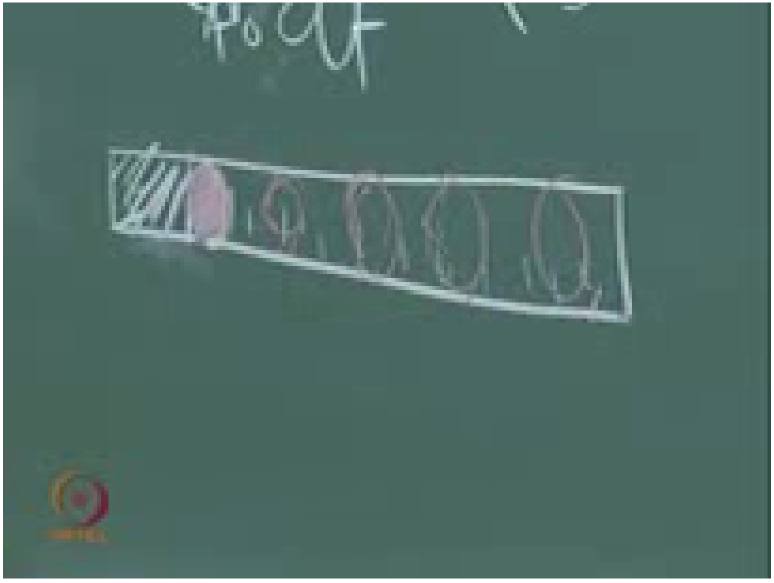
So then reaction starts and this is variable volume that means there must be mole change. Otherwise if there is no mole change this fellow will only sit there. He won't move. So because there is volume change, so it will try to expand and this will easily move.

(Refer Slide Time: 12:57)



Then it goes here in one minute, here. Ok. Another minute, may be here. Another minute may be here, Ok. Another minute may be here.

(Refer Slide Time: 13:21)

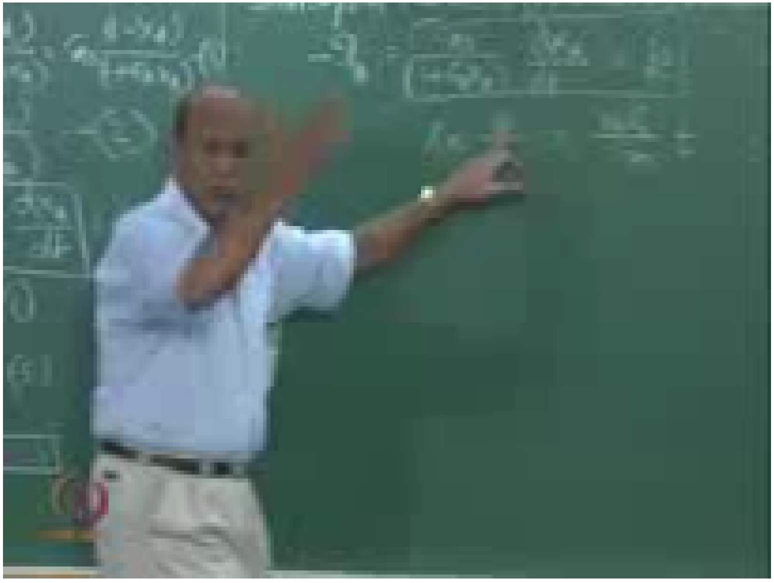


That means now you are trying to find out what is the length, you know cross-sectional area of the tube and then you can calculate what is V. What a wonderful, beautiful method as you know for engineers!

This is what what we have to imagine when we are now trying to do any experiment. I am not talking about only kinetics of any, you know any chemical engineering problems when you want to solve experimentally, you have to think all these. What is the easiest and the best method, what you can do, with the simplest one, as far as possible without costing much, right?

So I think these kinds of problems are there in Levenspiel, second edition also, wonderful book. All of you may be having only third edition. Go to library and then try to find out second edition, Ok. So actually he has given this kind of problems also. I do not know in third edition it is given there or not. Ok. So it simply expands, then we will record V,

(Refer Slide Time: 14:16)



V versus time. That is what what we are trying to do now, V versus time. So when I want to have my integral method, what I plot now?

(Professor – student conversation starts)

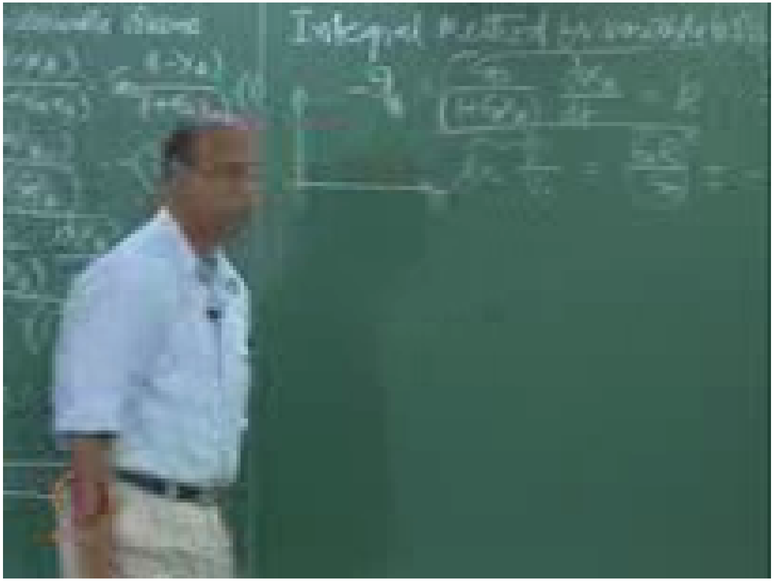
Student: Volume

Professor: Yeah, t versus

Student: Line 0:14:31.5

Professor: So I want to see that this is straight line so this entire thing as y, this is m, this is x.

(Refer Slide Time: 14:41)

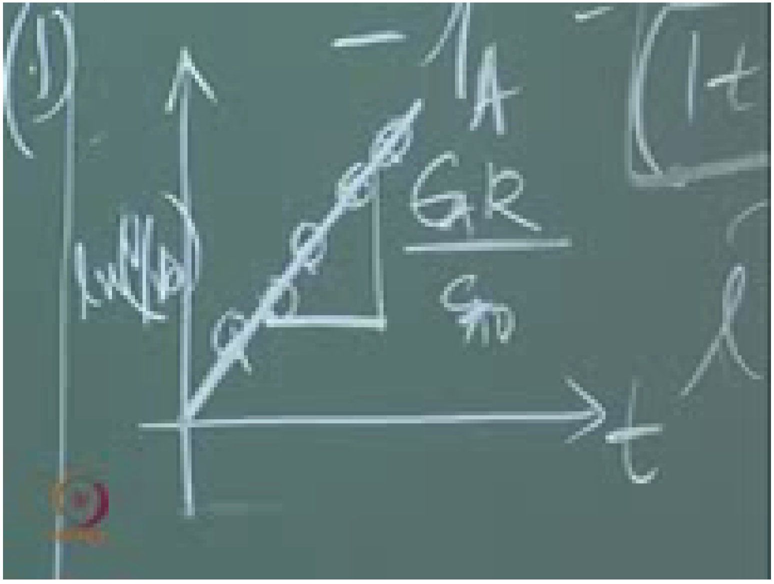


y equal to m x. So that means there is no c, so it should not go through, I mean it should go through origin, right, so then you will have... yeah like this. This is the one. Here I have to l n V by V naught versus T. So what is the slope now?

Student: epsilon A

Professor: epsilon A by k C A. You know epsilon A in the beginning itself.

(Refer Slide Time: 15:11)



How do you know?

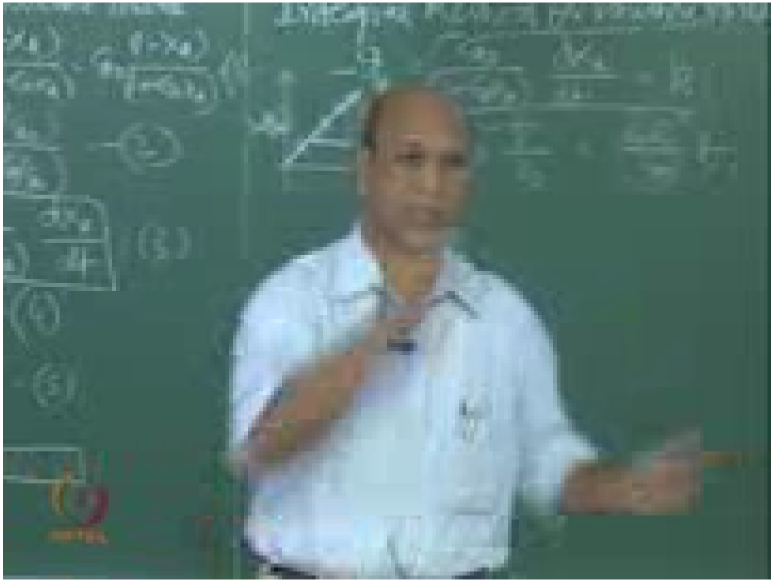
Student: From the stoichiometric equation

Professor: Yeah, either you can use your age old process like you know V at 100 minus V zero,

(Refer Slide Time: 15:21)

otherwise you can use the other equation where you know delta, delta A

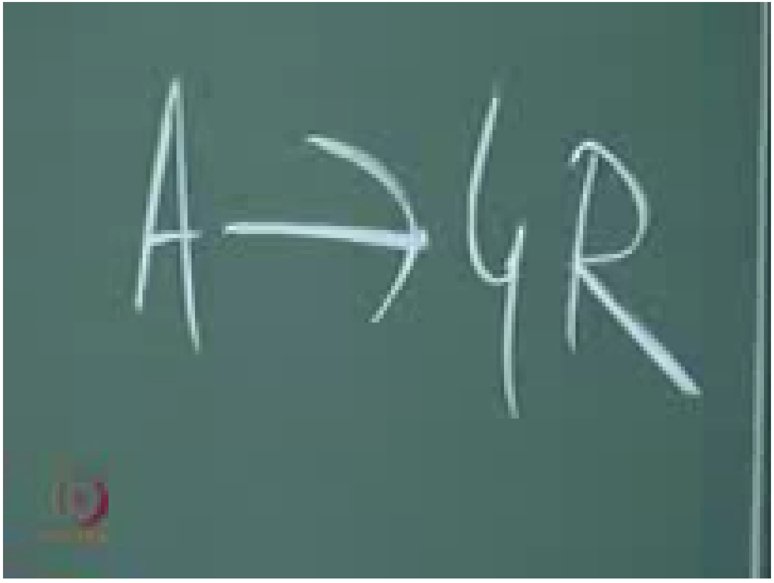
(Refer Slide Time: 15:26)



versus y A naught. If it is pure, Y A naught equal to 1, right? But only that delta difference will be there.

Delta is product's stoichiometric coefficient minus reactant's stoichiometric coefficient. If product is, let us say 4, 1 mole going to 4 moles, 1 mole Ok, using this, yesterday's technique, how do you find out? It is pure A.

(Refer Slide Time: 15:53)



Student: 0:15:53.6

Professor: Yeah, so y A naught equal to 1, and you have here 4 minus 1 by

Student: One fourth

Professor: No, no, not 4

Student: By 1

Professor: By 1.

R discussing

Professor: A no, delta N by

Student: A

Professor: You have to see, you have to be familiar with the equations, right. So A is 1, so that is how one can easily get. The moment I say I have 50 percent inerts, then?

Student: Into point 5

Professor: Into point 5. How much you get?

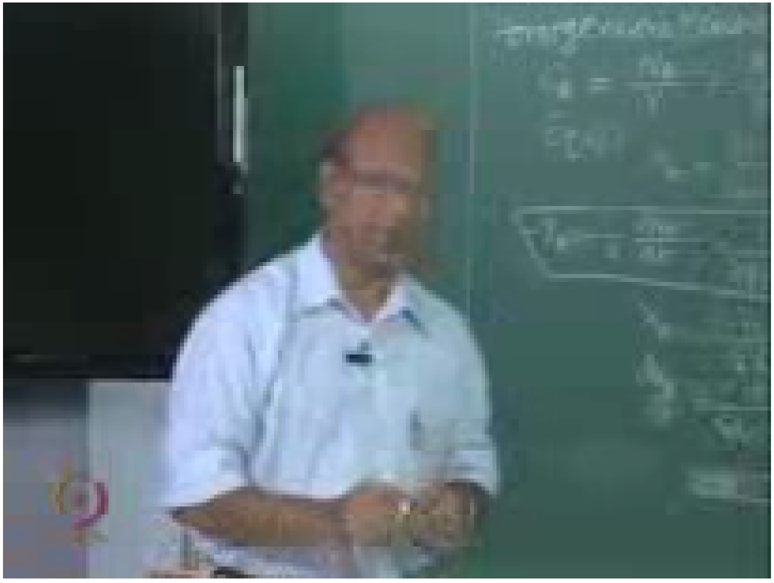
Student: Point 5

(Refer Slide Time: 16:31)

Student: Sorry 1 point 5.

Professor: 1 point 5, yeah now I am happy, Ok. (laugh). It is not only I make mistake, 0:16:38.5 also can say that. Ok. So it is

(Refer Slide Time: 16:40)



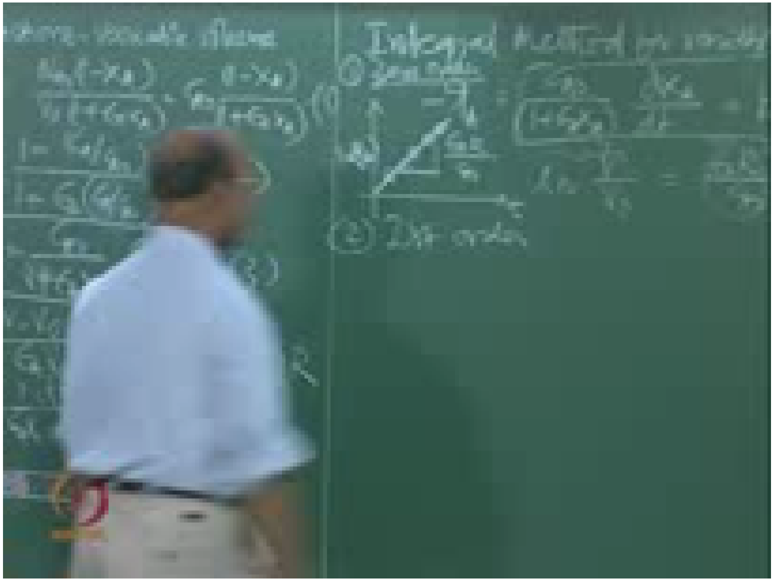
3 into point 5, 1 point 5, right, that is why it is also easy for us to find out.

(Professor – student conversation ends)

That is the reason now. We have taken the simplest example, simplest example and then I asked you to solve that. Now I will explain this one to first order reaction, right? Let us say that we have first order reaction. This is, Oh my God! I have not written here, zero order. Somewhere you write there, Ok.

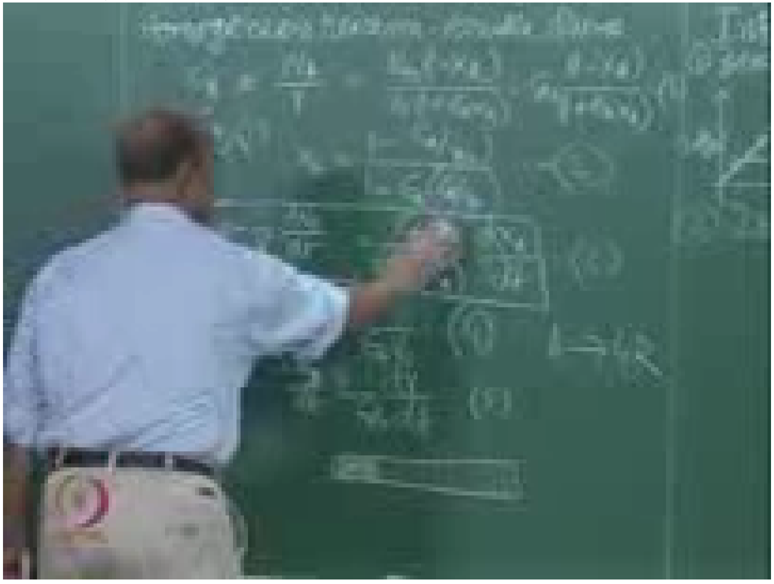
First one is, yeah next one is first order reaction.

(Refer Slide Time: 17:11)



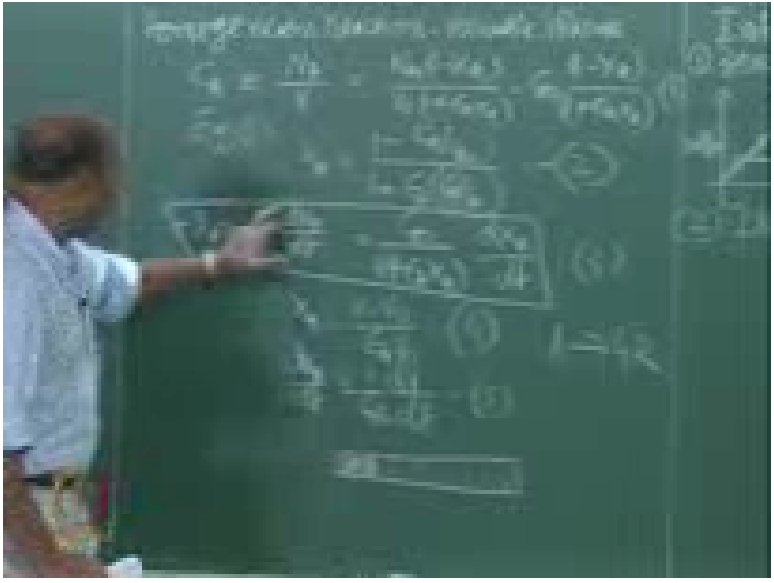
For first order reaction, again we will go to this definition,

(Refer Slide Time: 17:14)



Ok. So when I go to this definition, I have C A naught because I have already readymade, otherwise you have to write every time minus r A equal to this, yeah this one and write

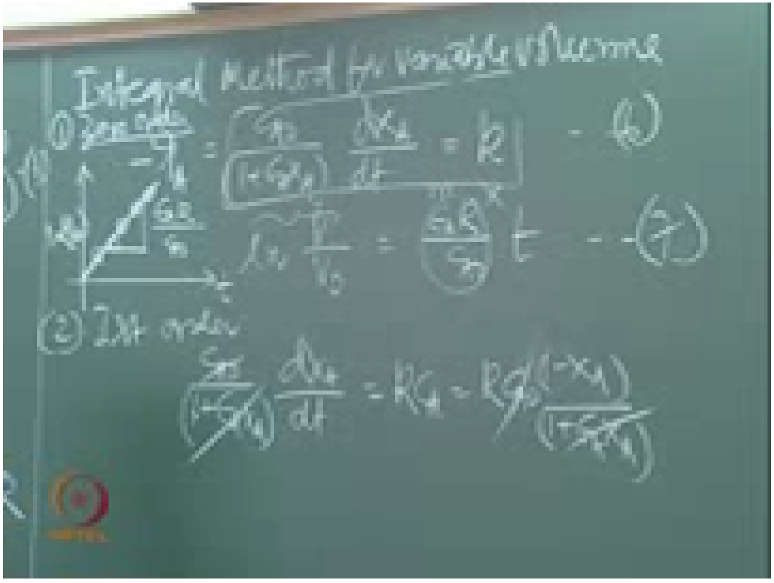
(Refer Slide Time: 17:29)



for V what is this and d N A by d T in terms of d X by d T, but already we have done so I am straightaway taking.

C A naught, 1 plus epsilon A X A, and d X A by d T equal to first order k into C A which is nothing but k into C A naught 1 minus X A by 1 plus epsilon A X A, Ok, good. Cancel. You can cancel out. And C A naught also goes, correct no? C A naught also, Ok. Now tell me, what is the

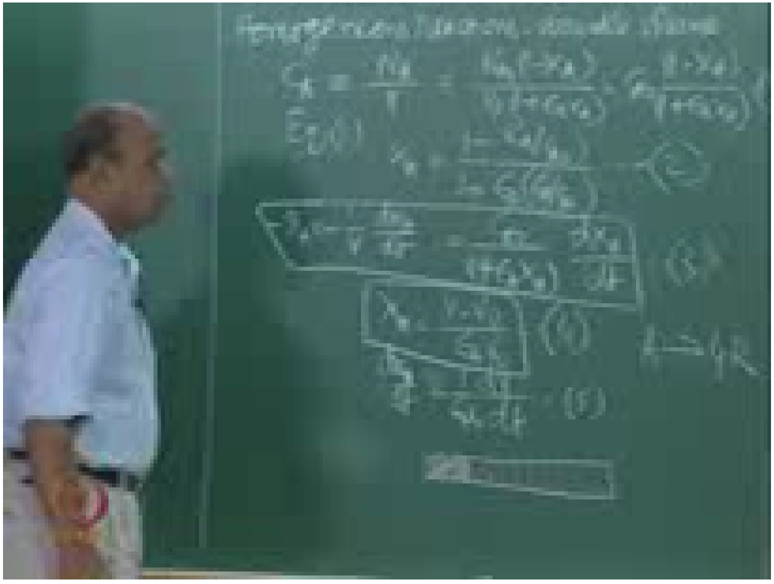
(Refer Slide Time: 18:10)



equation, integral equation for this in terms of again volumes?

Only thing is correspondingly you have to again substitute what is d X by d t and all that. And this side also you have to convert this 1 minus X A in terms of, I mean the volume. So X equation is this,

(Refer Slide Time: 18:35)



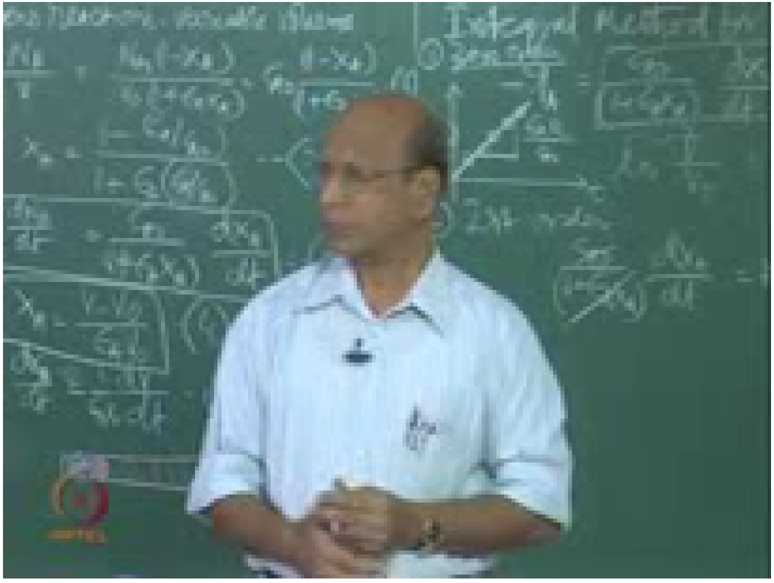
so you have to substitute for X. And also d X by d t, then integrate.

And someone tell me quickly, those who

(Refer Slide Time: 18:42)

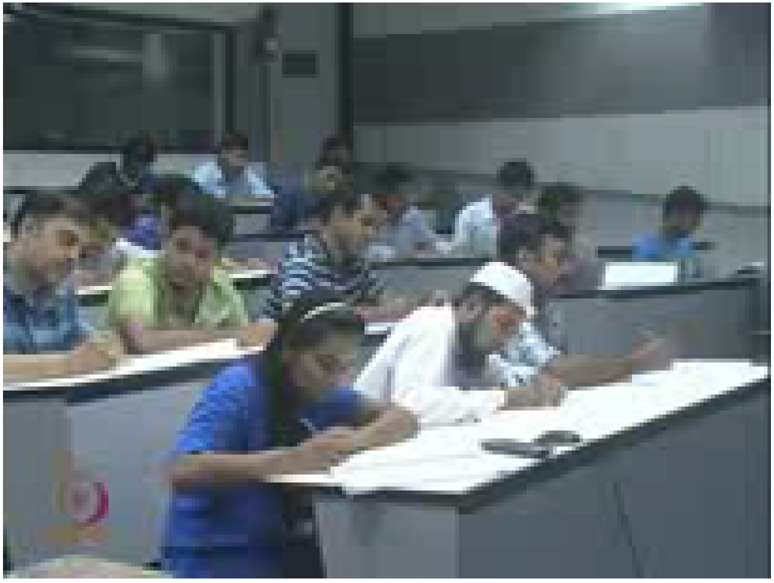
could not do here, I am sure they cannot do in the examination also. Right. That means you do not have that touch. I am not saying whether you are intelligent or unintelligent but only thing is experience. That touch is not there, practice is not there. That is why we have a beautiful saying, practice makes, yeah makes a person perfect.

(Refer Slide Time: 19:05)



(Professor – student conversation starts)

(Refer Slide Time: 19:06)



Student: l n

Professor: l n

Student: V by V naught

Professor: l n V by V naught equal to yes

Student: epsilon 0:19:13.4

Professor: Not so complicated. X i cannot come there. How can X i come? Because X i you are totally replacing. Because X i should be totally in terms of only V by V naught, anyone else? Yes 0:19:33.2. Tell me in terms of l n.

Student: I have not get that

Professor: You have not get that, you have to get the logarithm. There is another way, another simple way of doing also.

Student: Sir l n V by V zero equal to k T.

Professor: No, minus?

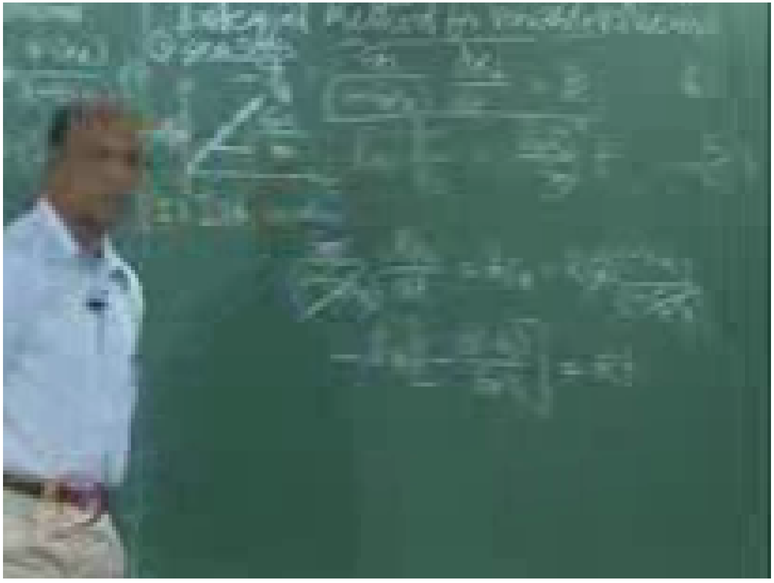
Student: l n of 1 minus delta V by xi into V zero equal to k T.

Professor: Excellent. That is the correct answer.

(Professor – student conversation ends)

Ok I will write here, you check, minus l n 1 minus V minus V naught by epsilon A V naught equal to k T. That is the equation.

(Refer Slide Time: 20:19)

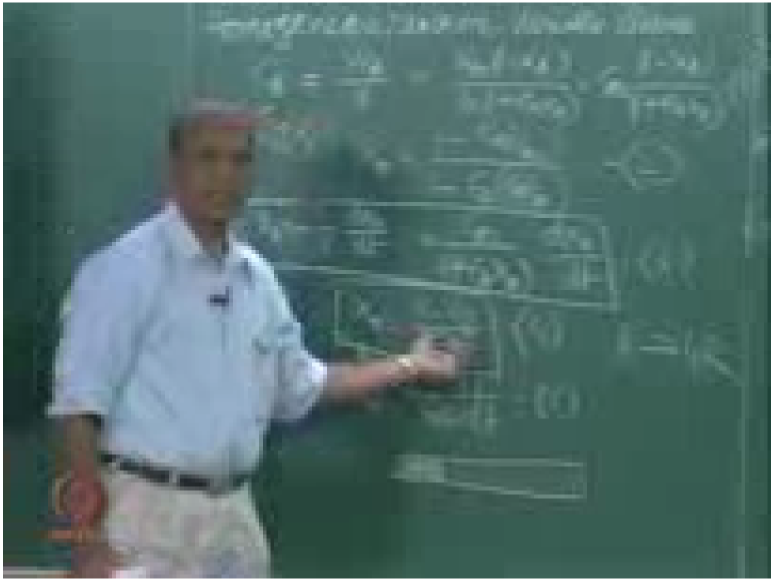


You would have made some mistake. Please check. This is why I am telling you, practice, practice, practice. That is the equation.

And I can tell you in a very simple way also, you know this equation. But I want you to learn through hard way. Ok. Yeah, what is the first order expression? As it is, if I want to, yeah so minus l n 1 minus X i equal to K T, what is X i?

(Professor – student conversation starts)
Student: X i is C A minus...

(Refer Slide Time: 20:49)



Professor: That is all. You see, one minute. That is how I give my surprise test. Yeah.

(Professor – student conversation ends)

So the another example is second order reaction which I do not ask you because 3 hours you may take. So that is why, this is second order reaction. We just give the integer expression in terms of differential equation. This is A plus B going to products, products where C A naught equal to C B naught.

Ok, that is again simplest case I am taking in fact. That means 1 mole, 1 mole C A naught equal to C B naught. That is the simplest case. So now what is the rate equation here? Minus r A equal to k into C A square, that is the equation. Right.

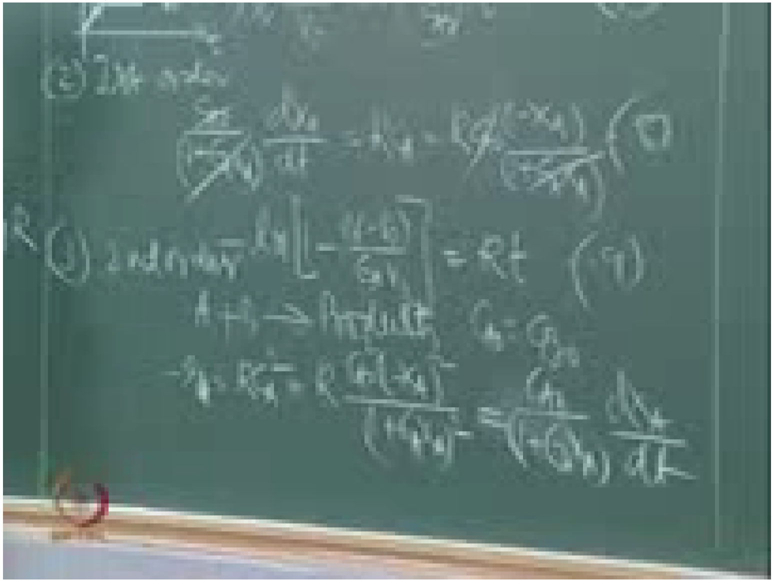
So this equation equal to k into C A naught square 1 minus X A square divided by 1 plus epsilon A X A square. It is a batch reactor we are talking all the time. So this is also equal to, this is 8, this is 9, this is also equal to what

(Professor – student conversation starts)

Student: C A naught 1...

Professor: Yeah, that C A naught 1 plus epsilon A X A into d X A by d T,

(Refer Slide Time: 22:14)

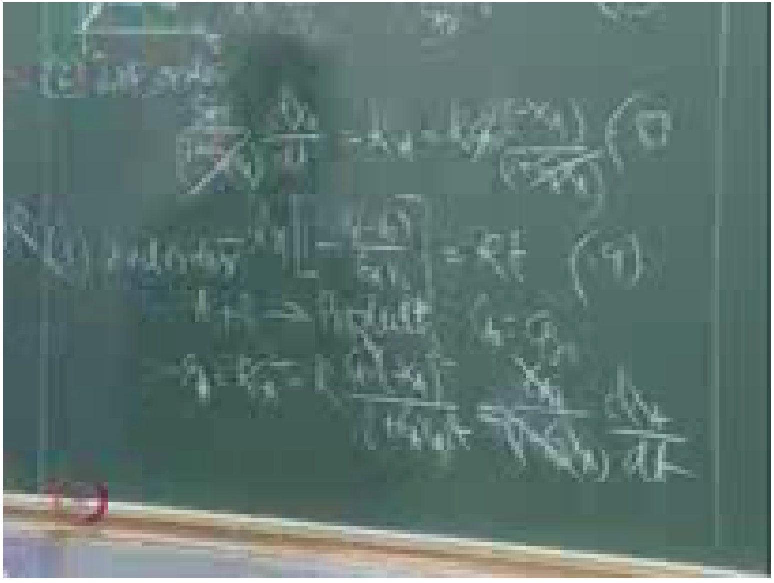


Ok.

(Professor – student conversation ends)

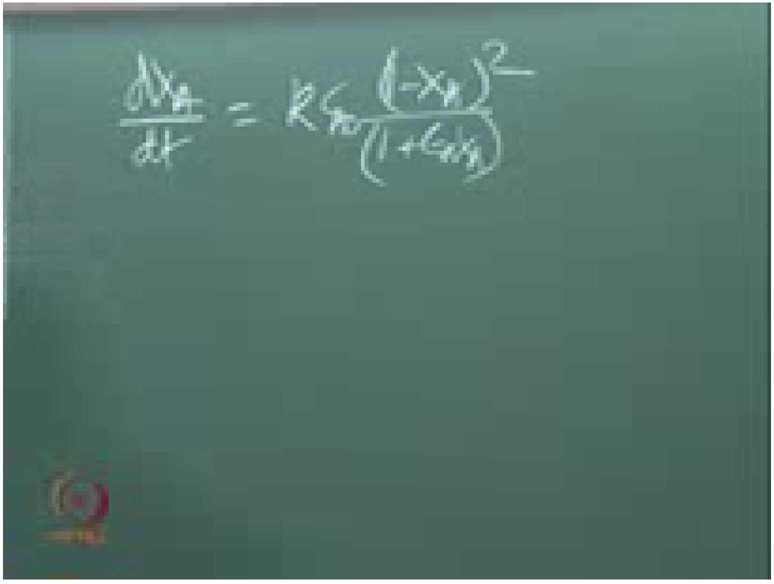
So what are the things I can cancel here? One C A naught I can cancel. And this side one epsilon A, no,

(Refer Slide Time: 22:24)



1 plus epsilon A X A also I can cancel. So now what is the differential equation I have to now solve? The differential equation will be d X by d t equal to, yeah this is equal to k C A naught 1 minus X A whole square by 1 plus epsilon A X A. So this is equation number

(Refer Slide Time: 22:55)



10. This is equation number 11.

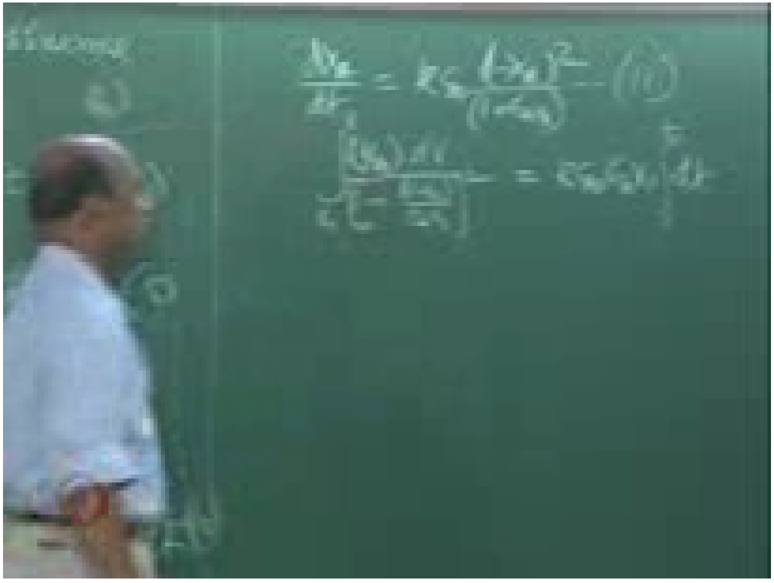
Now this is what you have to solve in terms of volumes, in terms of volume, right? Yeah. So now definitely if I give this one, may be next week examination also I do not think you can do unless you practice, practice, practice.

You have some techniques no, either substitution technique, this technique, that technique you know when you are solving this, when you are integrating. Ok. So that is why you have to use, you think, really all the techniques what you know till now and that is the idea of giving you mathematics course, no. Not for only just getting grade, Ok. So all that knowledge we have to also use in the real problems.

But I will give you the final expression. Final expression or just before final expression I will also give you that integral equation, in terms of V by V naught, please check me, sometimes I may make mistakes also, equal to 1 minus V minus V naught. I think you know some people can write V minus V naught as delta V, del V, I mean for simply, you know avoid more writing.

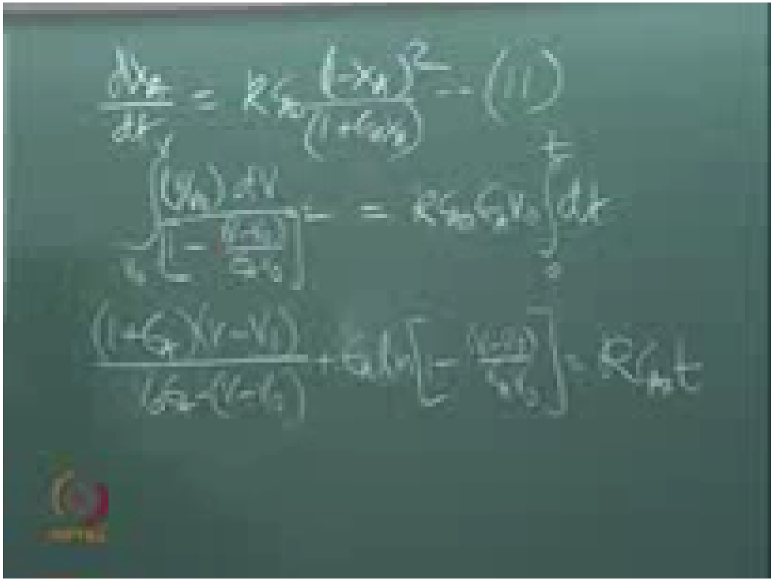
So this is, I am writing everything because, so that you can remember what is happening here, Ok. So whole square, this is square, equal to, because this one, equal to k C A naught epsilon A V naught into integral d t. So at time t equal to zero, it is V naught. At time t equal to t, this is some V, V.

(Refer Slide Time: 24:46)



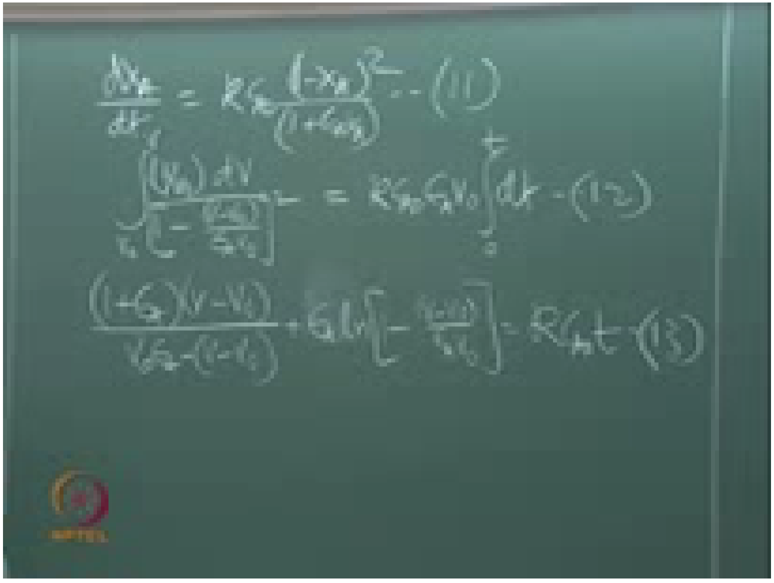
This is what you have to integrate. When you integrate you also get this kind of equation but please check again. V minus V naught by V naught epsilon A minus V minus V naught, yeah, plus epsilon A l n 1 minus V minus V naught divided by epsilon A V naught equal to k C A naught t.

(Refer Slide Time: 25:27)



So this is equation number 12, this is equation number 13. Ok. This is really complicated.
I do not think, I am not

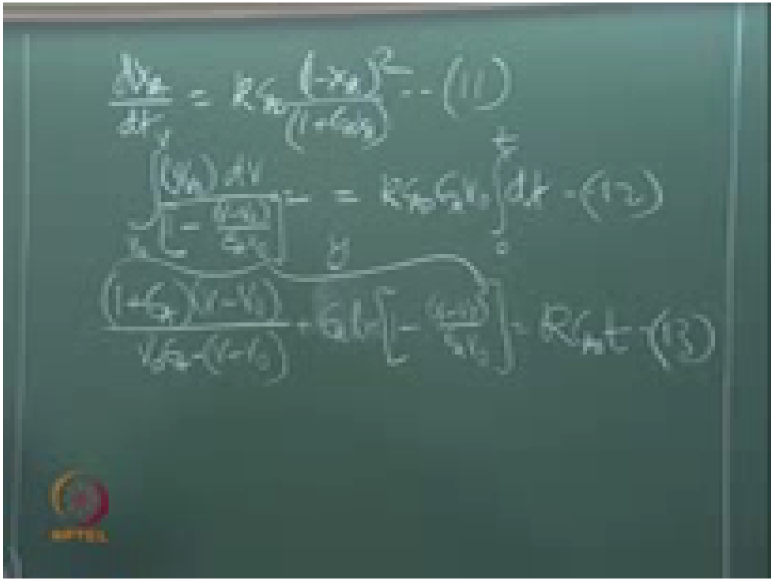
(Refer Slide Time: 25:40)



saying anything bad about you but only thing I am telling you is you need practice to solve this kind of problems. Once you have this equation, integral method when I am using, how do I plot this again? Because what do I measure? I measure V by V naught, or V. So V by V naught I know.

So that means this side, epsilon I know in the beginning itself. That is why I know all this side. So this entire thing I take as, straight lines are always better, curves are

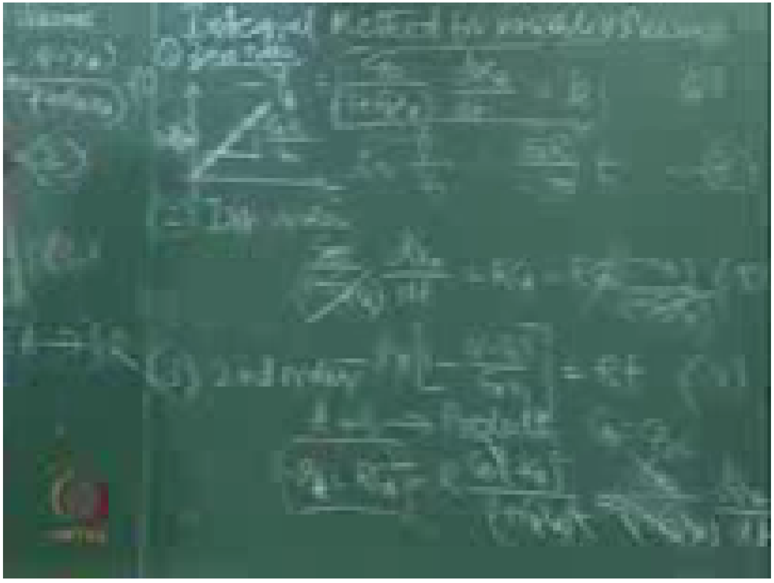
(Refer Slide Time: 26:10)



always dangerous. Ok, that you have to always remember. Curves are, 0:26:15.6, curves are dangerous. Because you do not know how the curves turn. So straight line, straight line you can easily see. Right?

So that is why you have to plot try as far as possible this as, entire thing as y and this one as m, t as x. Again y equal to m x. So that will go through origin and then you have to put, you know, all the, you have to put the points and then draw the line. And then you know if it is falling on the line then you are right, your second order assumption is right. So then you will have this one as the order of reaction

(Refer Slide Time: 26:52)



in terms of variable volume. Ok, good.

So I think I have given you the real difficulties in this, you know, integral method because integral method is the best method. But what is the difficulty? Because there is no free lunch anywhere. You have to work hard. That is why; you know there is no short cut for knowledge. Most of you won't realize that.

There is no shortcut, except you believe in Matrix movie. So there I think I have already told you also. Yeah, loading. Load C R E 1. Just go to I think, computer and then all C R E 1 problems, solutions everything is there, theory everything is there in your mind. If that is the world, I also would have liked it. It is really fantastic. But right now we are not in that kind of world, Ok.

So that is why practice, practice, practice. I am requesting you many, many times this practice. And that was the reason I gave you lot of problems. If I give one problem, no practice. Ok. So that is why if I give 100 problems, at least 50 problems if you do, that is practice for you. If you do 100 problems that is excellent practice. If you ask me 1000 problems, very, very excellent, you know for me, because that means you are real master.

And that mastery comes only by practice. You may be very, very, very, very intelligent person, Ok, very, very to the n, where n tends to infinity. You may be so intelligent, but still without practice you cannot do anything. This is life lesson. So that is why you have to. I think humans have not come to that level of, just looking at that and then you know again that Robot movie.

So this what I now want to sum up with the kinetics is that kinetics can be found out using either integral method or differential method. Those are not only two methods. And the remaining methods depend on your smartness. Like for example we also have what is called half life method. Ok, this is very smart method. But is it differential method or integral method?

(Professor – student conversation starts)
Student: Integral
Student: Differential method

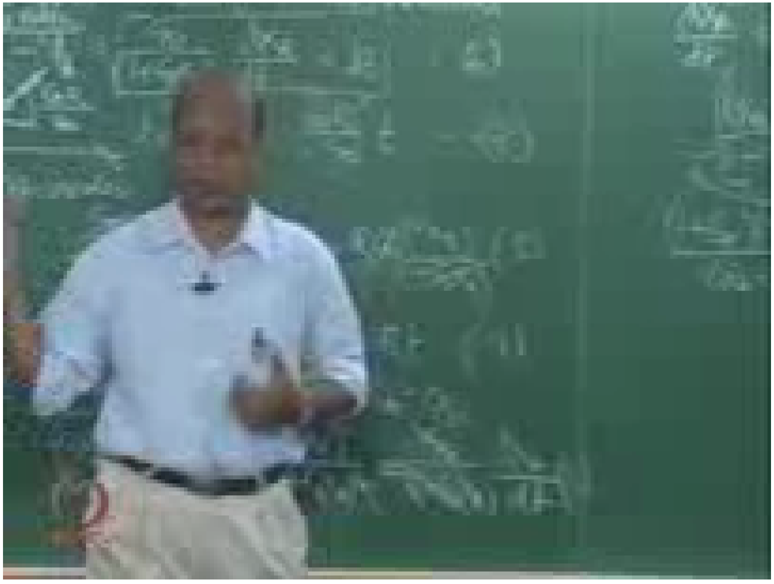
(Refer Slide Time: 29:02)

Professor: Both can be used, in fact.

Student: Both can be used.

Professor: Both can be used but the differential is very easy one because you assume now you have n th order reaction and then you will have, yeah for constant density system and that method is not that easy for

(Refer Slide Time: 29:18)

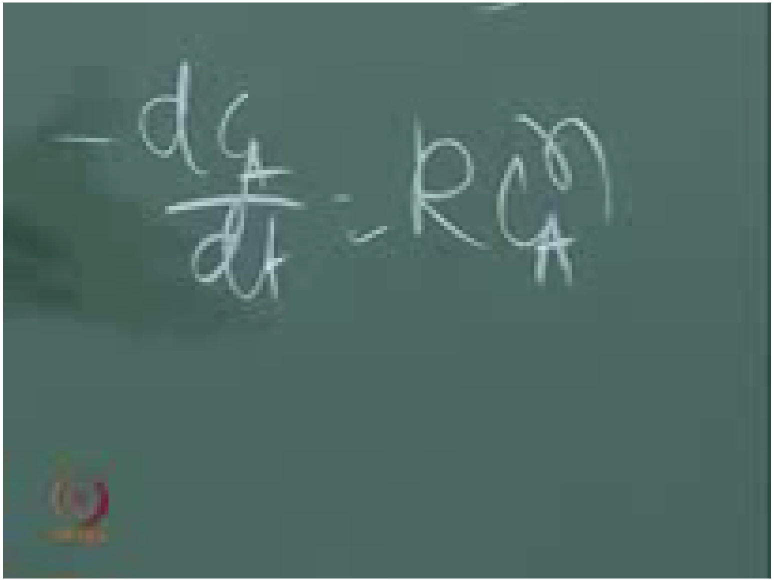


variable method, right.

(Professor – student conversation ends)

For constant density method, we have d C A by d t equal to k C A to the power of n.

(Refer Slide Time: 29:28)



Can I, whether I use this differential method or integral method, that is fine but I think, yeah, we are talking about only integral method for this, right? Why integral method? I will integrate this equation and convert this equation only in terms of only initial concentrations. How?

(Professor – student conversation starts)

Student: Sir C A equal to C A naught by 2.

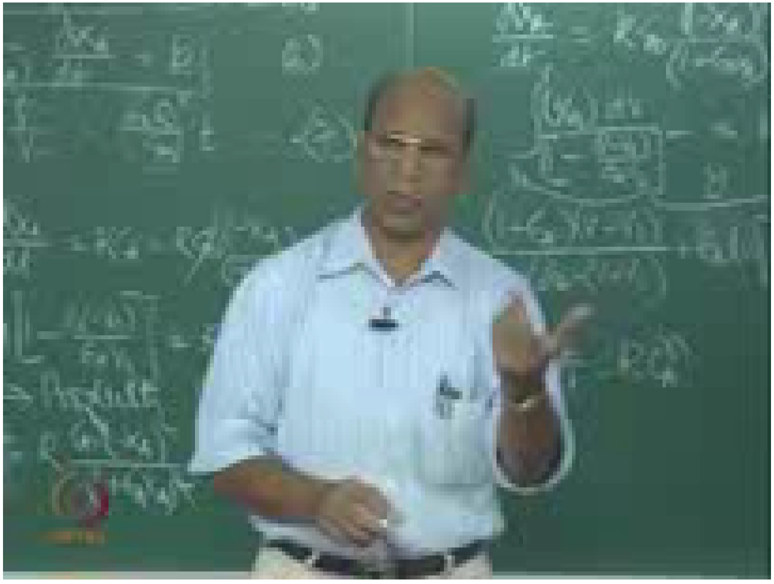
(Refer Slide Time: 29:52)

Professor: Yeah, that is the definition of

Student: Half life.

Professor: Half life. In fact it need not use half life.

(Refer Slide Time: 29:55)



It may be any life. It may be point 7 5 life. It may be point 8 life. Ok, need not be. But half life is very easy for us and half life started because of this radio, radioactivity so that is why half life we use very frequently.
(Professor – student conversation ends)

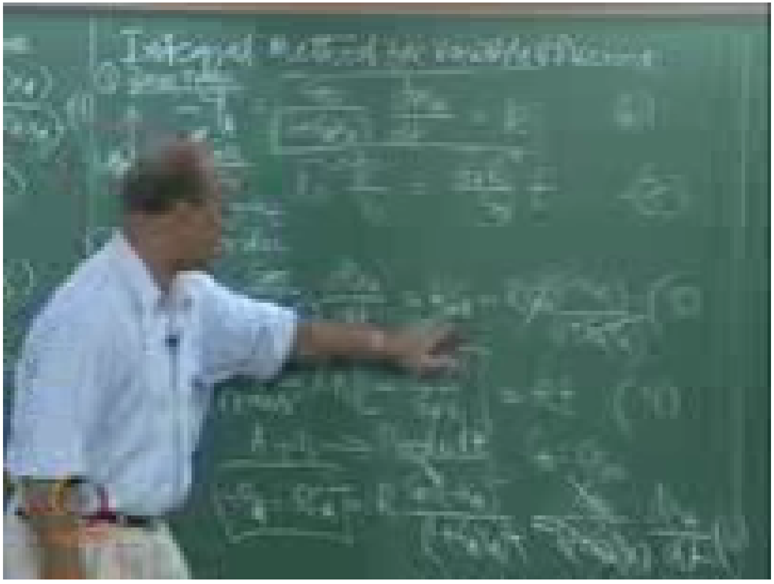
So then you will have only C A naught and time. Just C A naught and time, so that equation you have to plot. And I am not discussing all this because once you are experts in this, then your knowledge will increase and then you can use all these methods and your smartness will come out, what is the method you choose so that you can solve very accurately and very quickly.

So this is the method and then now, at this, at end of this discussion what we have now is A minus r A, whatever method you use. Ok. Whether variable volume or constant volume, right. So even though gas phase reaction, the number of moles are changing.

I may take a constant density reactor; batch reactor with closed, volume is not increasing or decreasing. No pushing like that. So then that becomes constant volume variable pressure reactor. So pressure is the easiest one to measure. Only thing is you should know what is pressure gauge. Ok, if you do not know that also you cannot run that.

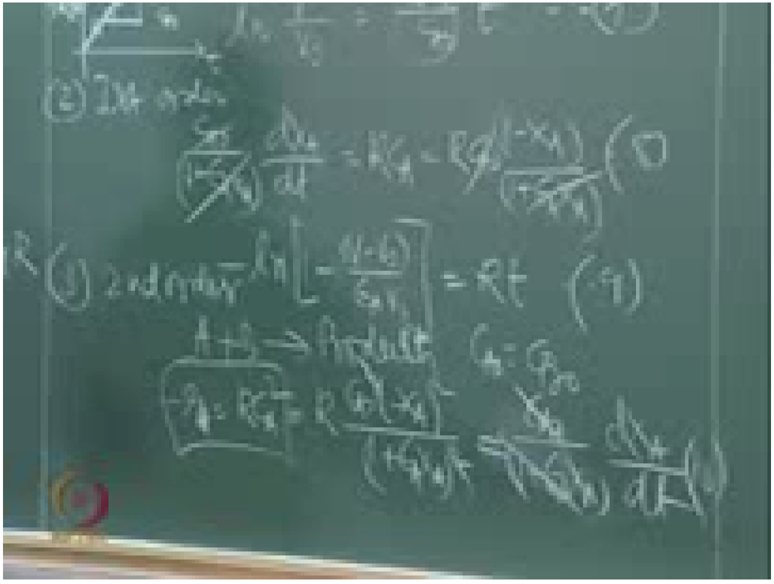
So take that and then measure pressure and then go to that equation which I gave no last class and use that partial pressures and again come back here to write this kind of equation where minus r A,

(Refer Slide Time: 31:22)



this C A is nothing but P A, right but only thing is when I write this C A in terms of P A, then k by R T is a new constant for me.

(Refer Slide Time: 31:31)



So that is why I think that you have to take care of with correct units and you know, correct dimensions. All that you have to take care of. Otherwise the method is same everywhere. But again I tell you, it depends on your smartness.

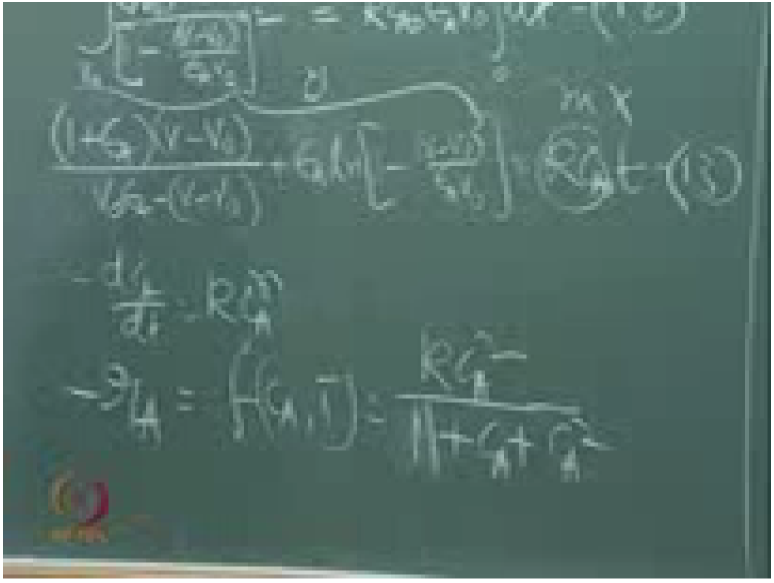
Particularly those people I think M Tech people may do coursework and then some project and leave but I would like to see, if I am here, I think by next June I will be out, but I think before that if you are able to do something very smart please tell me, I will be the first man to be very, very happy. To see that, yeah this is a very smart idea, right?

That smart idea that is what we seek from the student. Ok. That smart idea is nothing but how simply you can do within shortest time. That is what the smartest idea, right? That is what the smartest idea.

So that is why; please remember that at the end of all discussion we have what is called minus r A. This minus r A is simply, can be a function of simply C A and t. It can be as simple as k equal to; I mean minus r A equal to k C A square.

Or it can be as complicated as k C A square by another capital, no I think, capital K if I write, you may take it as equilibrium, so m plus C A plus C A square.

(Refer Slide Time: 32:54)



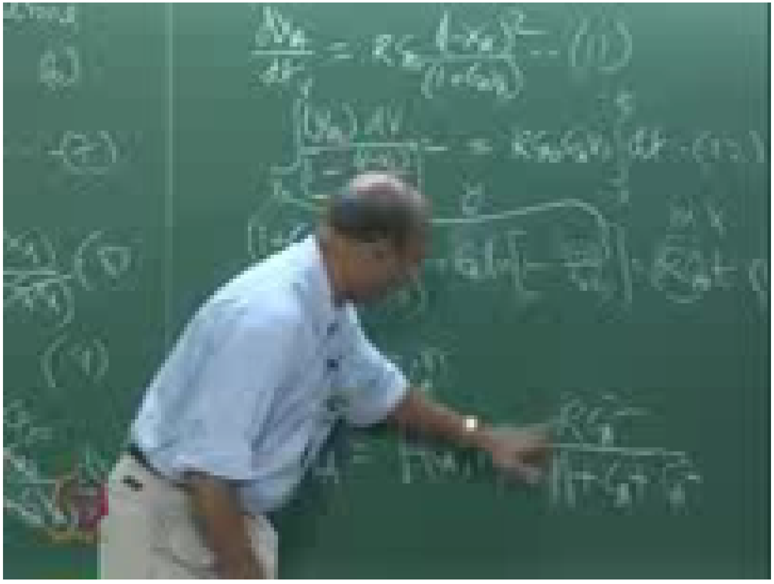
Now just imagine. This is equation which I have to use here for finding out the rate also. Somehow I found out and then this is the kind of equation what we have, right?

So even this equation also, what I can write here is this is minus r A. I get the minus r A data, right. That means imagine that we have constant density system. I am telling all simple things because easy for you to visualize.

Next one is only difficult things where you have to, you do not have to use your brain there but only you have to be careful in using mathematics, that is all. Mathematics come there only. But conceptually it is same, right? Now again I have to plot this one as a straight line. How can I do that? If it is possible.

Otherwise if it is not possible, then what I do is I turn this way. 1 by minus r A is equal to this by this. Now I will have

(Refer Slide Time: 33:46)



each one dividing. So that means I have something plus something plus something. Now that is easy for me to solve. Instead of this equation where it is as it is.

So that is why all these smart things will come by practicing. So this is the one what we have. It can be, yeah, one thing what you have to remember is this minus r A is no more order of reaction. If we are very, very lucky only you will have first order, second order so that kind of specified orders, right? Otherwise it can have any form. That is what.

That is why do not say that minus r A equal to k C A to the power of N but say that minus r A is a function of C A and temperature. And there is no other function. And there is no other variable which is changing rate. I mean of course, sometimes catalyst may change but we are not talking about catalytic reactions, that is postponed to next semester, good. Ok.

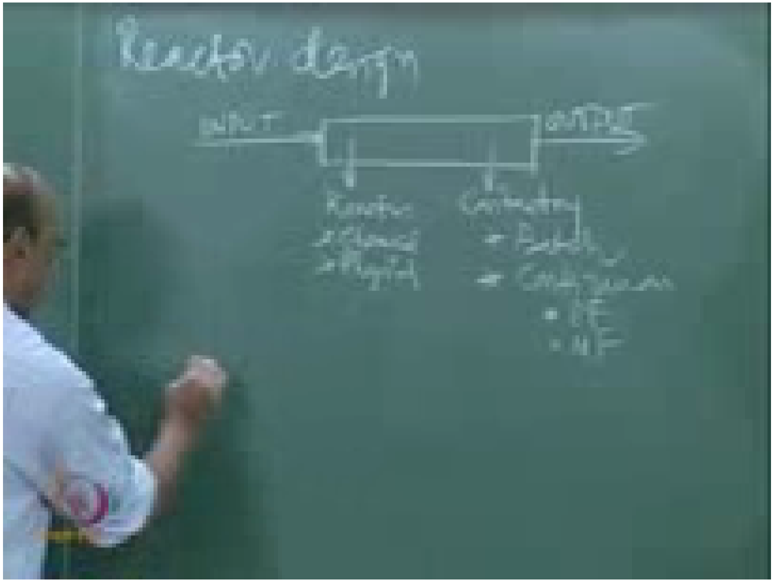
So now using this information what is our next thing what we have to do. So now I will start

(Refer Slide Time: 34:44)

with my diagram. So of course, reactor design we go back again. Information required is this. Output, input, kinetics, contacting, so here I have chemical, yeah chemical, physical or physical I have written first, Ok, so this is one, stars, batch, continuous, and in continuous you have P F, M F.

So we are very happy to have only three here, all three together.

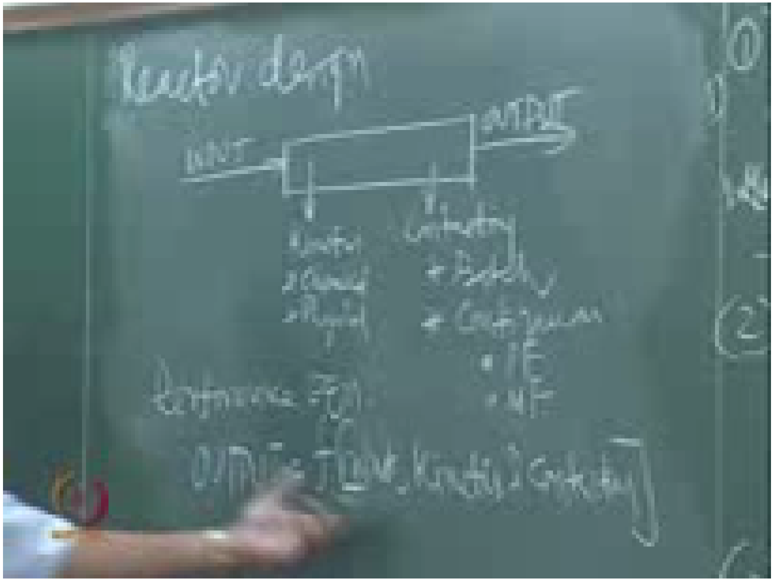
(Refer Slide Time: 35:42)



So then we have output performance equation, You know, this is a nice word, performance equation. Ok, sometimes you feel, Oh very nice word but I think performance equation is nothing but design equation for that, for us, Ok. What is the final design thing what we are trying to do?

So output is a function of input, kinetics and contacting, yeah that is the equation. Now do you have all these terms? That means output is a function

(Refer Slide Time: 36:23)



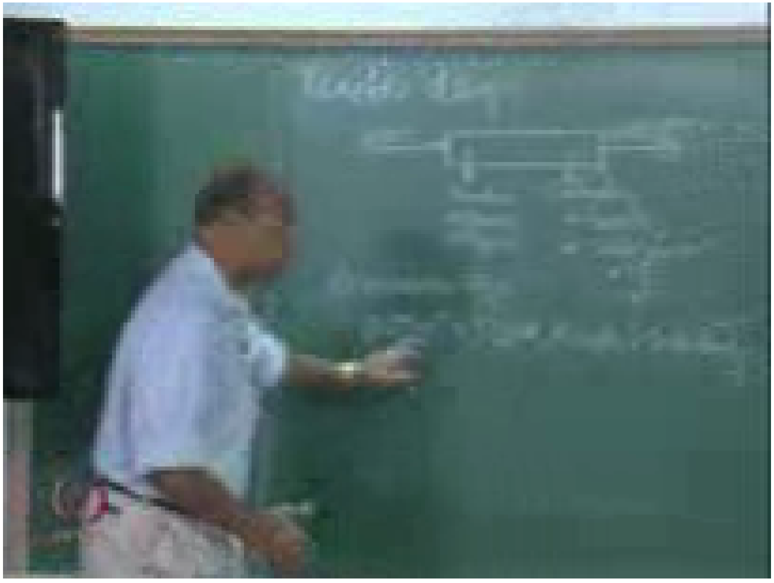
of input, kinetics, contacting, like here rate as a function of concentration and temperature, right? So this you understood. What is the functionality of rate with respect to T, temperature?

(Professor – student conversation starts)
Student: Arrhenius
Professor: Arrhenius equation
Student: Arrhenius equation
Professor: Right, that is all. Only one you have, very easy.
(Professor – student conversation ends)

But most problematic parameter is function of C A. It can be anything. You do not have any choice with you. But whereas with temperature you have at least one choice, it is, I think proved till now that that is the only best equation that can be used for finding out change of rate with respect to temperature, Ok.

Similarly here, I have now output. That means if I want to design a new reactor, Ok, I should be able to find what, volume. If I have a old reactor and then I want to find out again

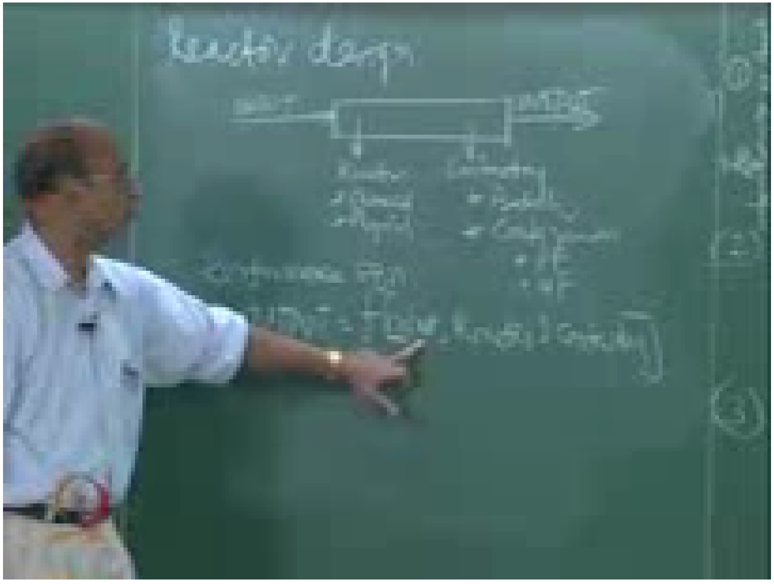
(Refer Slide Time: 37:17)



output what is the output from old reactor, existing one? Conversion. That is all. The design problem.

So now we assume that we have a new plant and then I am going to design the new volume, Ok for the reactor. So that means I should know output,

(Refer Slide Time: 37:32)

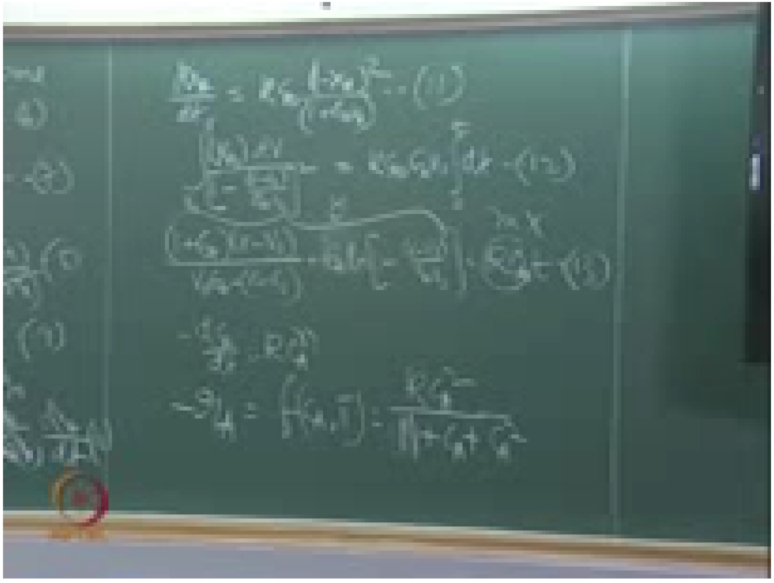


that is how much you know, we have to send to the reactor then I should know kinetics,

(Refer Slide Time: 37:38)

kinetics is nothing but minus r A, some form of that f of C A T, some form.

(Refer Slide Time: 37:46)



If you are lucky, that may be simple first order reaction, k into C A.

Then the other thing is yeah, contacting. So contacting also you have an idea. Right, contacting will tell you, contacting will tell you which design expression you have to use, please remember that. Ok. Contacting will tell you which design expression, there are three design expressions.

So one is the batch reactor, you know when you have to choose. And the other two are continuous reactors; you also know when to choose. So if I say that Ok, I need, design a plant for me for 10000 tons per day, very large, Ok so our mind will automatically go to continuous.

So continuous I have again two, so what is that, where my mind has to go in the next step?

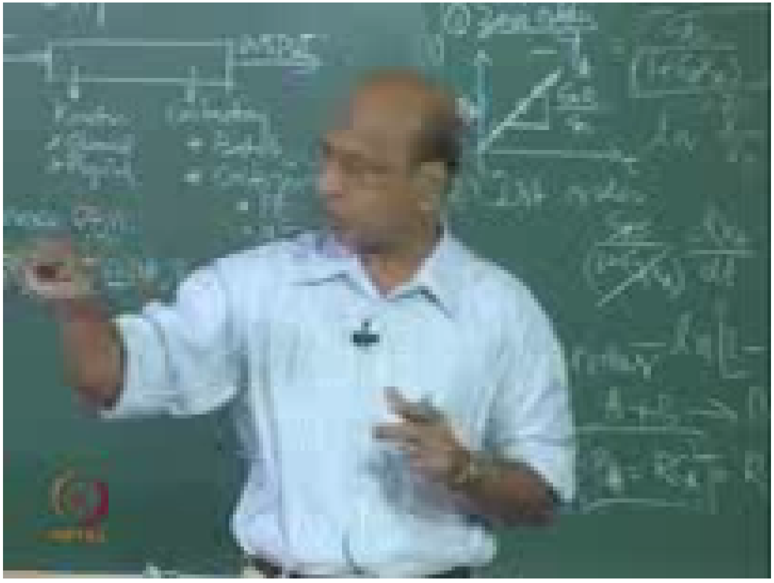
(Professor – student conversation starts)
Student: Depending on
Student: Plug flow reactor
Professor: Why plug flow reactor? By definition plug flow reactor is always

(Refer Slide Time: 38:34)

Student: 0:38:35.6
Professor: efficient for n greater than
Student: 1, zero
Professor: Zero. Zero, all positive order reactions, n greater than zero, Ok
(Professor – student conversation ends)

And if you are not believing that, just draw 1 by minus r A

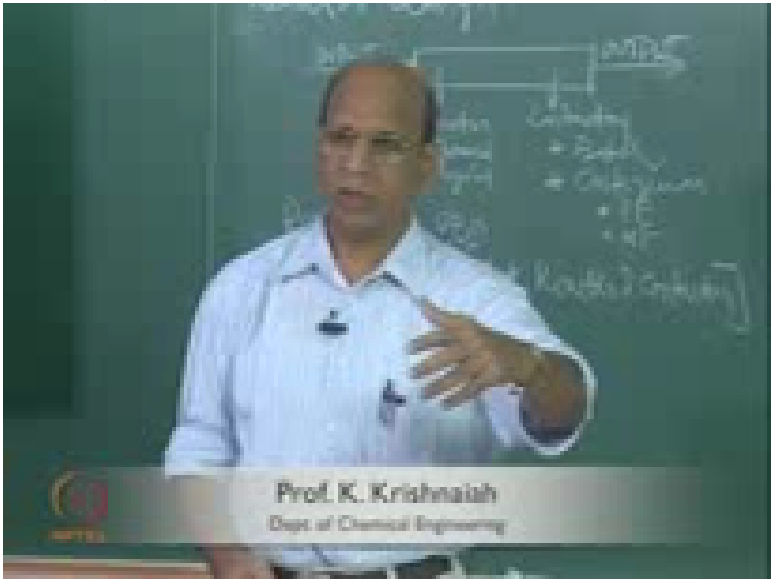
(Refer Slide Time: 38:48)



versus X A, 1 by minus r A versus X A, and then see which one will give you lowest volume, area, lowest area, Ok. That is one of the easiest methods to find out the arrangement of reactors and all that. Ok. Instead of worrying about remembering n greater than 1 and, normally all n greater than zero, the plug flow reactor is the best reactor.

But we do not use all the time. Why? Because if it is exothermic reaction then temperature is crucial. If temperature is crucial, I will go to mixed flow in spite of, in spite of you get more conversion for small volume

(Refer Slide Time: 39:32)

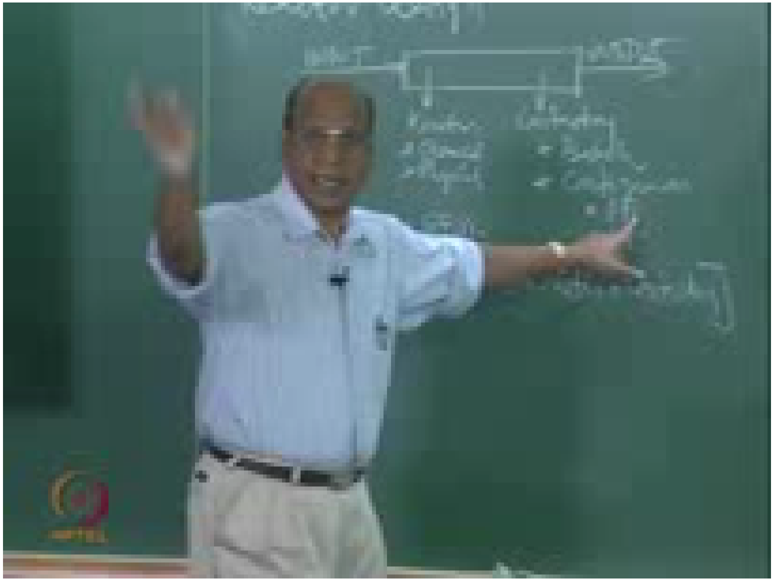


for the reactor. In spite of that you know, so this is always the correct thing no?

When you know that this guy may be highly intelligent, super intelligent but he is always a trouble maker, will you hire him in your organization? 0:39:47.9 will you take him and live with him with all the problems? So you do not. That is what. You know that he is excellent, his brain is super. But still we do not. The reason is that we want to compromise. We want to have smooth operations in your plant.

That is what exactly the choice between plug flow and mixed flow because I know, plug flow for all the reactions

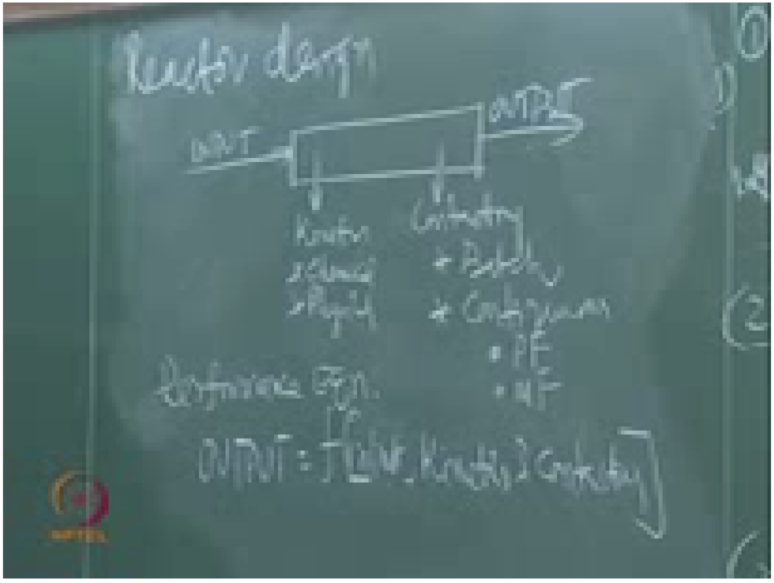
(Refer Slide Time: 40:10)



n greater than zero, definitely plug flow will be best. But still I will see that whether I have to live first, Ok to operate the reactor.

So if I take the plug flow and if the temperature is uncontrollable, explodes who will run the reactor? There is no reactor once it explodes. So that is the reason we go for the mixed flow which is very easy to control

(Refer Slide Time: 40:30)



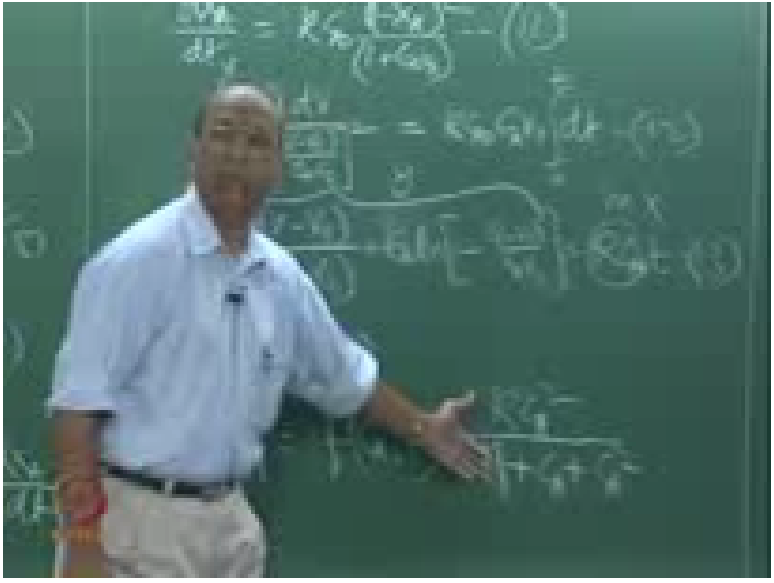
and temperature, one temperature you can maintain by definition.

So that means, contacting also you know how to choose. Kinetics also you have to choose, I mean you know how to get. And input you know that is the simplest one what you get. This is what is entire reaction engineering; that is all. Now you have clear idea what is minus r A and how do you get it. Ok, including heterogeneous systems.

Because I gave some examples. If it is coal burning how do you get the rate? If it is catalytic reaction, simplest one, Ok, I have not done Hougen-Watson model Ok, but that I will do next semester. But that method is also exactly same. Approach is exactly same. You will get minus r A slightly complicated like this.

I am talking

(Refer Slide Time: 41:13)



about Hougen Watson model for heterogeneous catalytic reaction, Ok. You remember that form, minus r A equal to P A minus P B into K divided by, in the denominator you have 1 plus something, 1 plus something you know, like that you will have. That is a complicated equation. But approach is same, exactly like slurry reactor.

Slurry reactor you have so many steps. The other two at least we have taken only two steps because irreversible and all that. But you also know, at this point of time, how do you get a rate for heterogeneous system. That means you have all that information. I am not exaggerating. That is the information, basic information that everyone should know in any reaction engineering course.

Now next onwards, it is only the details, details, details and slight combinations. That is all what you have to learn. Otherwise you do not have to learn any new concepts, right. But something. You know even if I say recycle reactor it is a combination of mixed flow and plug flow. Because it is intermediate mixing between plug flow and mixed flow, right.

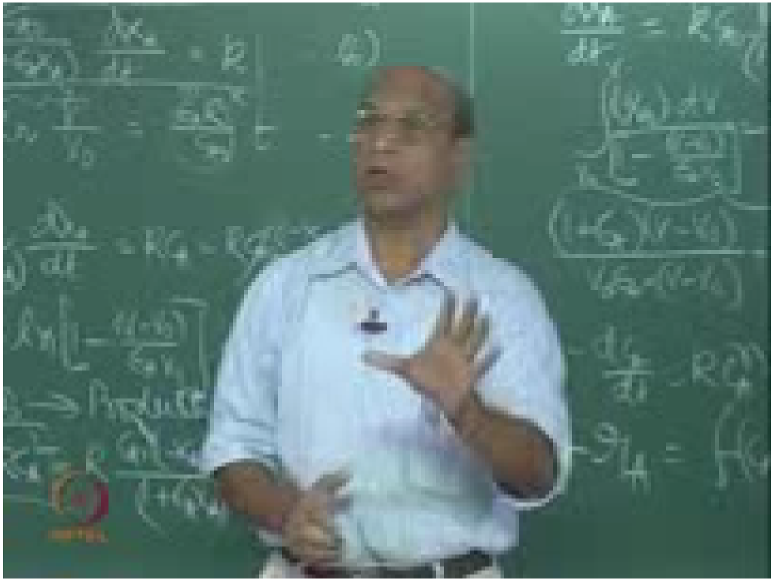
I mean other thing I can tell you is, Ok, I take now 5 C S T Rs in series or 2 C S T Rs in parallel. And one C S T R in parallel and another C S T R, sorry C S T R is M F R Ok, Ok, one M F R

(Refer Slide Time: 42:37)

in one branch and another P F R is another branch, Ok, how do you get? All kinds of manipulations only what you have to learn.

And it is not easy also

(Refer Slide Time: 42:47)

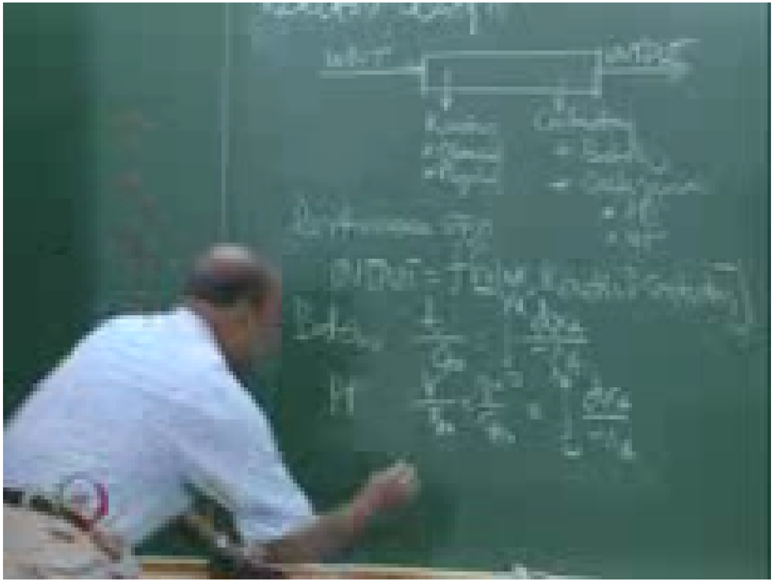


because it involves mathematics. And mathematics require practice. Ok, yeah if it is, take practice. Like this only you have to. Otherwise it is not possible, right? So that is why the next thing what I do is combination of reactors.

And just before going to that, some people have still some uncomfortable feeling with the difference between tau and t bar, Ok because we have now taken individual reactors and thoroughly seen.

But we have 3 equations, for batch, it is t by C A naught equal to zero to X A d X A by minus r A. And for P F, V by F A naught which is unfortunately written as t by, tau by C A naught, correct no, can be written, equal to zero to X A d X A by minus r A. And other one is

(Refer Slide Time: 43:48)



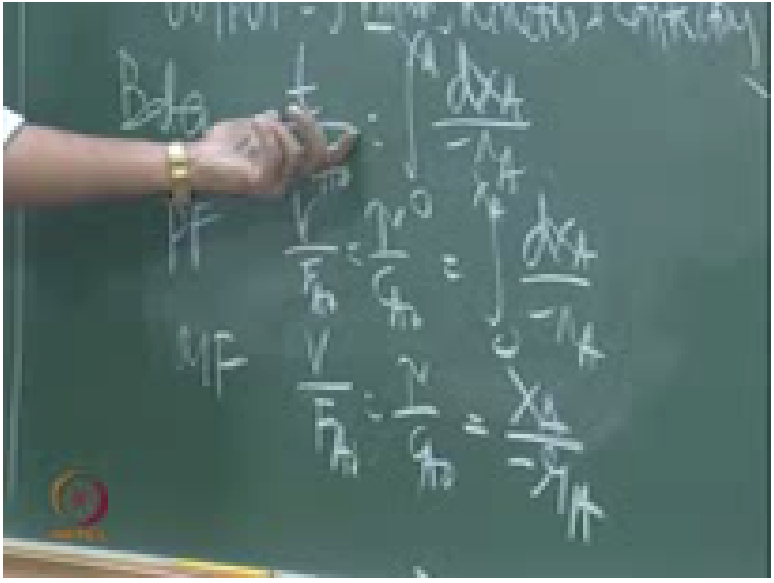
M F, is V by F A naught also equal to tau by C A naught X A by minus r A.

These things you have to remember, right. Yeah

(Refer Slide Time: 44:05)

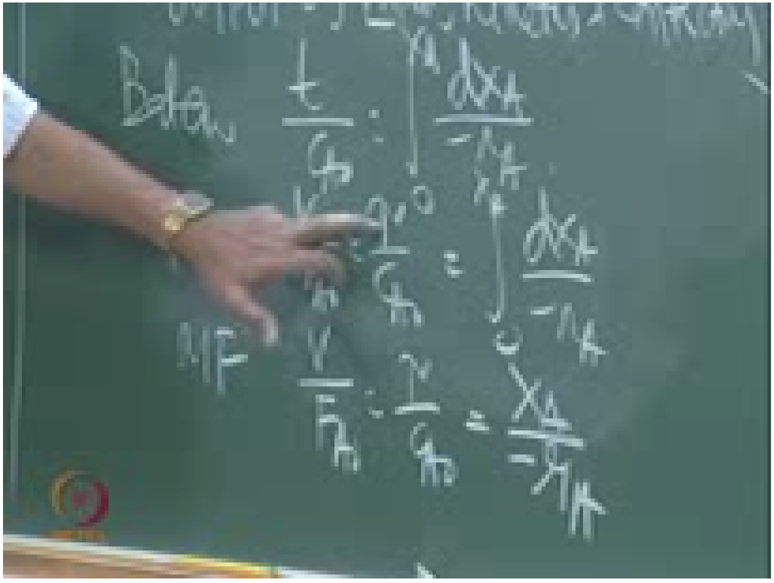
and unfortunately the first reactor what you have learnt, the batch reactor

(Refer Slide Time: 44:09)



is having this format, t by C A naught, Ok. So that is the reason why we would like to also express

(Refer Slide Time: 44:18)



this tau for the other two reactors. That is the only reason. Otherwise you do not really require for design.

See in the design, what do you do, I say? You would either find out conversion if volume is given. So volume is, I know here. Ok. Or otherwise find conversion, sorry, find volume if I know conversion. That is all what you do. So that is why, why tau is required?

But I think we should have some psychological feeling that we also know tau and also sometimes it is easy to write in terms of tau rather than V by F A naught, right, yeah V by F A naught. That is the reason why what we have, good.

And I will ask you this question, what is the natural time that automatically comes in the design? Is it tau or is it t bar? We are telling t bar is the mean residence time where it is defined as the molecules pending, you know some time, on the average, t bar no, mean residence time, on the average what is the time spent by the molecules inside the reactor. That is t bar, the time spent by the molecules on the average inside the reactor. And space time...

(Professor – student conversation starts)
Student: Volume
Professor: We know, I think space time is you know it is time taken to process one volume of
Student: Reactor volume

Professor: Yeah, one reactor volume. And we also have another complicated thing, the space velocity, the reverse of it.
(Professor – student conversation ends)

Unless we are blaming our, we are loading our C D, Ok, or hard disk. So that is why I think you know all those things are not required as far as I am concerned but still we need that because sometimes you can write very simple equations in terms of k tau, like del, you know del. del is the simplest form of writing complicated equation.

Similarly sometimes k tau will be a parameter where you can nicely put it and k tau also has a number called Damkohler number. So again I think to respect Damkohler we can also learn what is k tau. But my question is what is that naturally coming one? Naturally coming time in the design. He says t bar, I am not saying he is right or wrong, Abdul right or wrong. But I mean, what is your opinion? What, that means naturally it has to come. You do not have to do anything else. Naturally it won't come.

Naturally it has come means it has come in the equations without your, any problem. Without any extra effort. That is why Levenspiel nicely uses a word, natural performance measure. Time for example if you take, what is that? Natural performance measure. Is it tau bar, is it t bar, or tau?

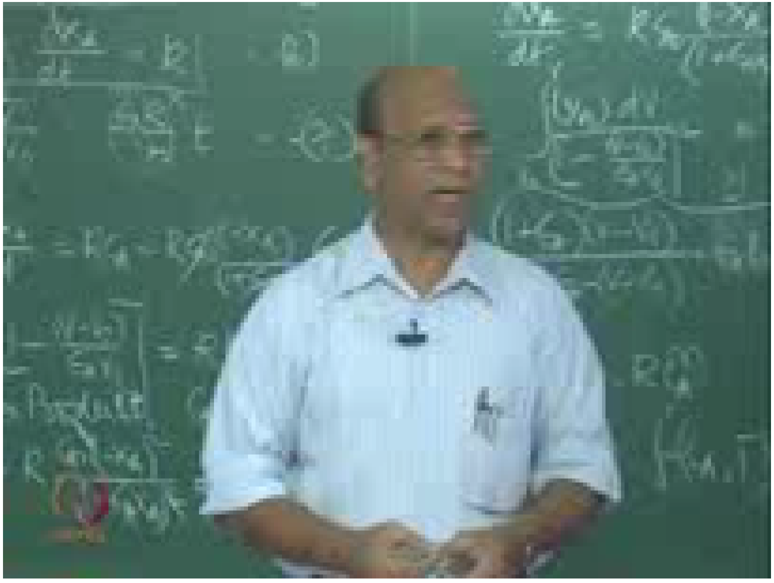
You know the difference no, tau is defined as volume by volumetric flow rate where the volumetric flow rate is mentioned at the entry, correct no, at the entry. Whereas t bar is the time on the average, actual time on the average that is spent by the molecules inside the system. Which is the natural measure, t bar?

(Professor – student conversation starts)
Student: Tau
Professor: Tau, yeah, Rajshree, in-between? You said something, tau? Why do you say tau is the natural measure?
Student: Because it is coming directly from the equation.
Professor: Yeah, actually

(Refer Slide Time: 47:33)

tau is the natural measure of; you know performance for any reactor. Why?

(Refer Slide Time: 47:38)

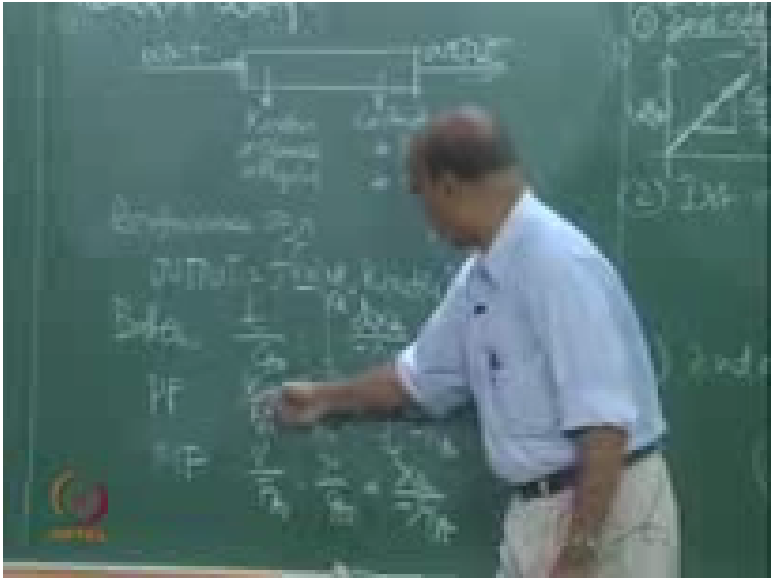


Because it is coming naturally in the material balance equation.

(Professor – student conversation ends)

Because what I did, this V by F A naught, I know what is the relation between you know,

(Refer Slide Time: 47:47)



volume by volumetric flow rates, C naught, F naught and all that, that is why simply I substitute. I have not done anything extra there. But whereas t bar to find out is not that easy. And unfortunately this natural measure will not give me a clear picture.

(Professor – student conversation starts)

Student: 0:48:02.1

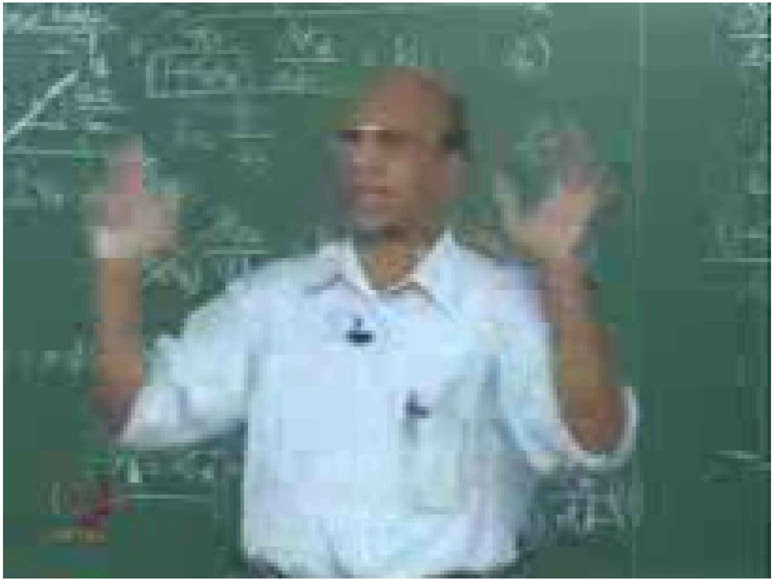
Professor: Yeah, but why do you want to check? Because it is not coming in the design. Why do you want to check? You do very well in examinations. The moment you know this chapter I am not focusing, Oh it won't come, do not touch. Ok but why do you want to know t bar where you are not using anywhere? Where are you using t bar unless in the examination if I ask you, find t bar?

(Refer Slide Time: 48:24)

Student: 0:48:26.7 perfectly, it is better to use t bar than tau?

Professor: Where do you use? Where do you use, tell me. Because what is the, what is the aim of this

(Refer Slide Time: 48:36)

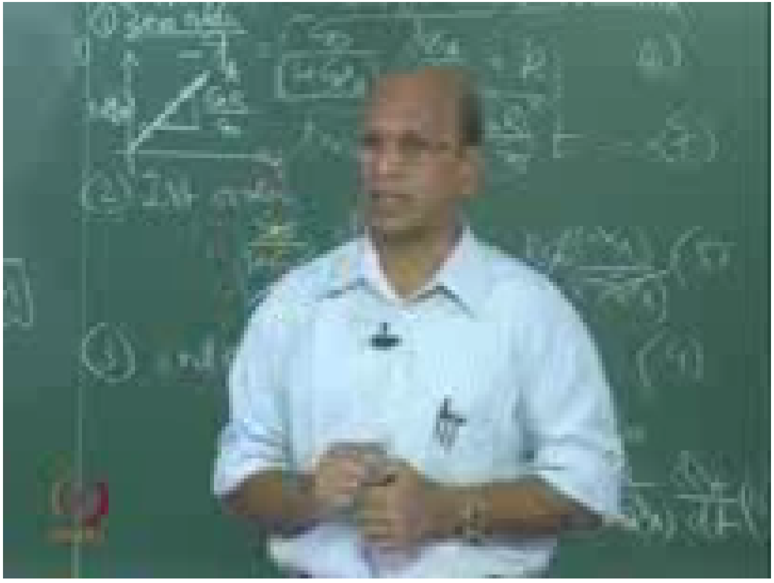


entire reaction engineering? To design the reactors,

(Refer Slide Time: 48:39)

Ok.

(Refer Slide Time: 48:40)



To find out the volume of the reactors. Where is t bar coming, you tell me. Even non-idealities where is t bar coming there?

(Professor – student conversation ends)

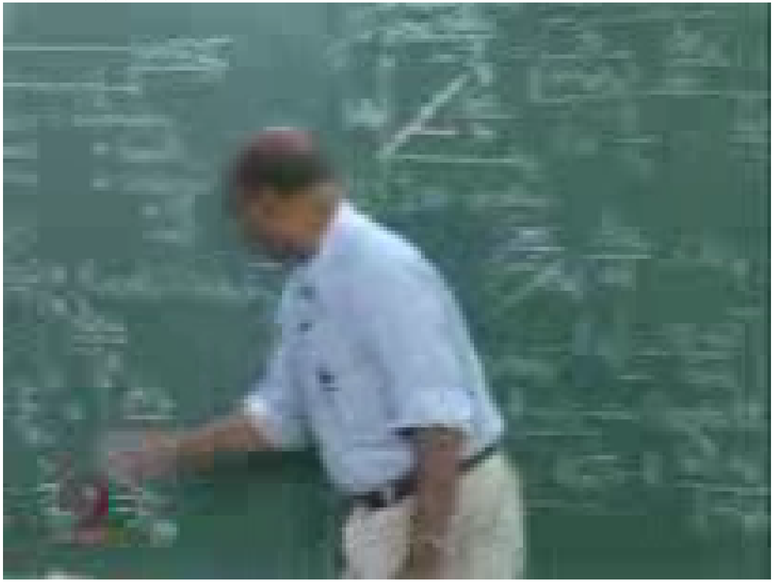
For the design I am talking, actual design. There also what you do is you try to measure the amount of non-idealities. For example if I have dead space, Ok, I have 1 meter cubed volume. I would like to find out out of that 1 meter cubed, that means 1000 liters, out of 1000 liters, how many liters are in dead space, not very actively participating. That is all what I want. Why do I need t bar?

One way of find out that is t bar, that is Ok. So that is different. So that is why as far as we, you know, design is concerned, particularly these ideal reactors, 99 percent of the time you go for only ideal reactors. Non-ideal reactors we do not go.

The reason is particularly the mixed flow is very easy to manage. We get almost perfect mixing. So I have the simplest equation. right. And plug flow, normally for gas phase. That is why gas phase reactions we use, the flow rates are very fast, the reaction timings are very fast that is why you will get almost flat velocity profile, you are sending at very high Reynolds number through the reactor, right? That also can be managed. And maximum thing what you can add there is axial mixing. There also we do not go for dead space and all that.

So that is why we are only in the ideal world. Or very close to ideal world. So that is the reason why t bar and tau, where you have to, I am telling all this because I am not against t bar or tau. What I am telling is when I am naturally trying to find out what is the volume or conversion, from the design expressions where I have written material balance and all that, t bar is not coming at all.

(Refer Slide Time: 50:13)



It is only the tau which is coming. If you want to use tau. Actually that is also not required. Why? V by F A naught directly I can get. Ok, good. But in spite of that

(Refer Slide Time: 50:40)

I may ask you a problem in the examination

(Refer Slide Time: 50:43)

or sometimes you write you know k tau, k tau, tau is very easy, Ok to find out because volume by volumetric flow rate but you have to specify what is the point at which this volume is defined.

You know you also heard of what is called of liquid hourly space velocity L H S V, liquid hourly space velocity.

(Refer Slide Time: 51:01)

Space velocity of course is inverse time, Ok. So that is not the point. But why we use that is, again engineering simplification, right?

So you have actually vapor phase reaction, good? But before making this vapor we have only the liquid form, the liquid. Then we vaporize, then it becomes vapor and then enters into packed bed or may be plug flow reactor. Or may be C S T Rs. Ok. Depending on the temperature. So at that time when you are doing it, for me easiest measure for me is particularly in industry is liquid. Right.

So you now send some 1 liter or may be 10 liters or 100 liters which is corresponding to that flow rate which is just entering the reactor, Ok. But actual basis is this equation where? At the entry. At the entry, but you are not considering that. What you do is, Ok how many liters I will now flow through the rotameter. Liquid, because it is available in the liquid form.

Then afterwards it goes to the heat exchanger. From heat exchanger it goes to the reactor. Now I have calculated what is that vapor velocity that has to enter at that point or F A naught. That is V by F A naught. That comes there. But instead of remembering that one, I will now remember that is equivalent to how many liters of liquid.

That is what it is called. If you are able to convert this time in terms of liquid velocity, then it is called you know liquid hourly space velocity. Now it has become old fashion. No one is using that. Similarly gas hourly space velocity, so that means somewhere else you measure.

See normally at room temperature it is very easy to measure. All your rotamotors and all that, at room temperature. Why?

Maintenance is simple. It is at room temperature. I do not have to worry, you know suddenly putting my hand and then burning, jumping. Because at room temperature if I am able to flow, make the gas flow this I will remember but actual entry is at may 300 degrees Centigrade, 400 degrees Centigrade. What will happen to gas? Gas will expand. I will calculate, that is my basis.

For the reactor design, that is the basis. Not this. But for me to remember, to operate this is the easiest. That is why industry people will try to remember those things much easier. I do not know whether you noticed or not, I mean when I first came to Madras, I noticed, I mean I am a lousy observer, that is my problem. Because once I observe, 99 percent of the time I am right in my observation, I am not wrong.

You know, looking at people and then trying to find out, and I also like each and every small detail, small things. So when I came here first, you know, there are the Mount Road and you know, our transport is bus only. And you know, in the bus stop people will stand. One person will come out there. He will say like this. Ok, and all other people will be waiting for the bus to stop.

So then afterwards, I think I observed some 4-5 times and afterwards I just asked someone why only he is doing like this and then all other people are standing there. It seemed that is the signal to driver that he is from P T C. The person who is doing this is P T C guy.

So even if it is not stop, because you know all buses may not stop in that particular stop, all the buses. So that is why if he says that, he will at least go forward and then stop. This guy will go, run and then climb there. That is the signal because that is the easiest one for them.
Similarly in industry also, we have some thumb rules. Liquid. Actual reaction is vapor phase.

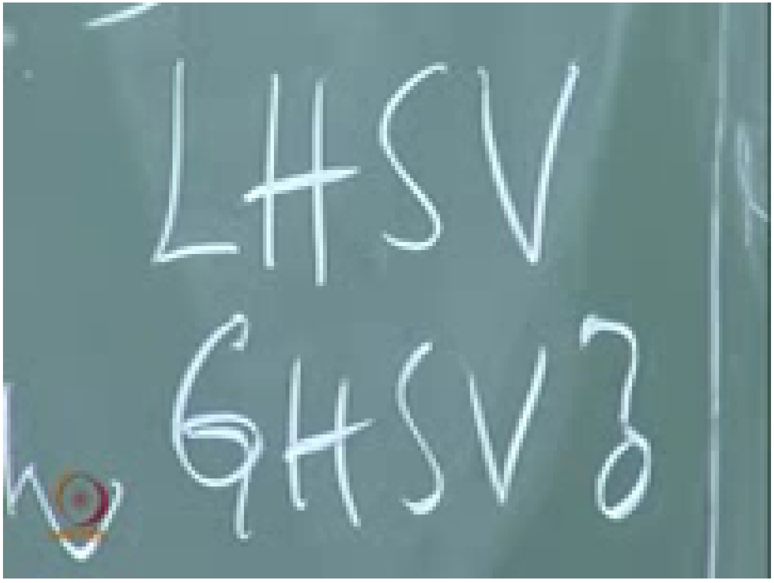
But he knows that, by doing this, liquid for him. So that is why I think there are some.
I think in even railways also they will say that Ok 47 Down has gone, he will say. Example. 47 Down, it is only numerical value for us. 47 Down. But he knows 47 Down may be

Coimbatore Express. Ok. That means his actual name; he is trying to convert into the simplest language which they can understand much faster.

That is what exactly the meaning of L H S V and also I think G H S V, this is question mark, I am not exactly remembering. L H S V. So that is why it is only convenient because suddenly there are many books nowadays in reaction engineering.

Many books have come, last 10 years. So that is why some books, also industry people have written, not academicians. So that is why they may be using these terms still.

(Refer Slide Time: 55:38)

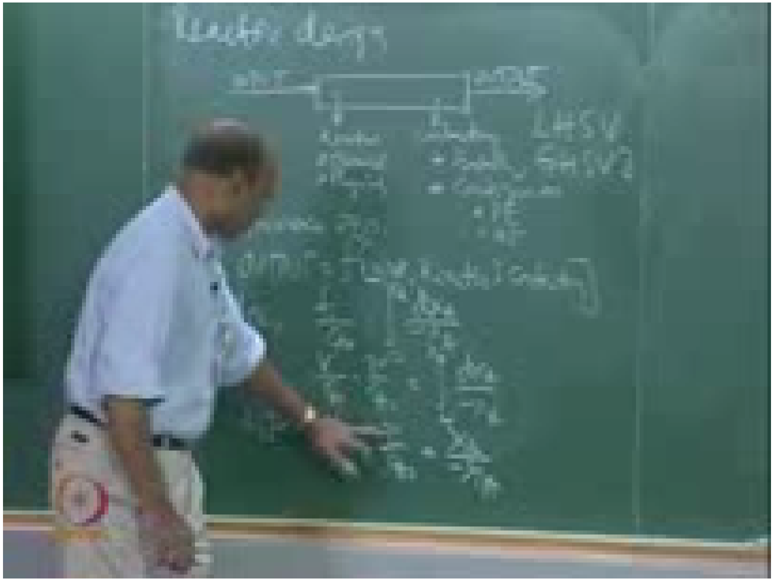


So if you are able to see that, do not get confused.

And V by F A naught is only the correct one, Ok where this F A naught is the actual one which is entering. Mass will not change, Ok. So only the velocities will change depending on you have volume, large or small, depending on what temperature you are sending.

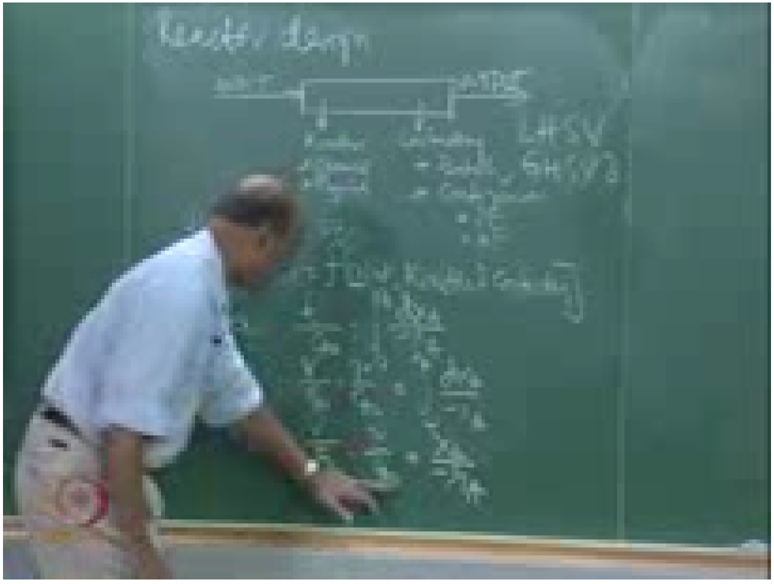
And if it is liquid, reaction also taking place in liquid phase. It is a constant density system. Again whether you measure here or there or anywhere it must be same, volume also. Mass is same, Ok, good. So this what.

(Refer Slide Time: 56:10)



And tau you know, how do you find out, Volume by volumetric flow rate. But that volumetric flow rate normally is V by V naught,

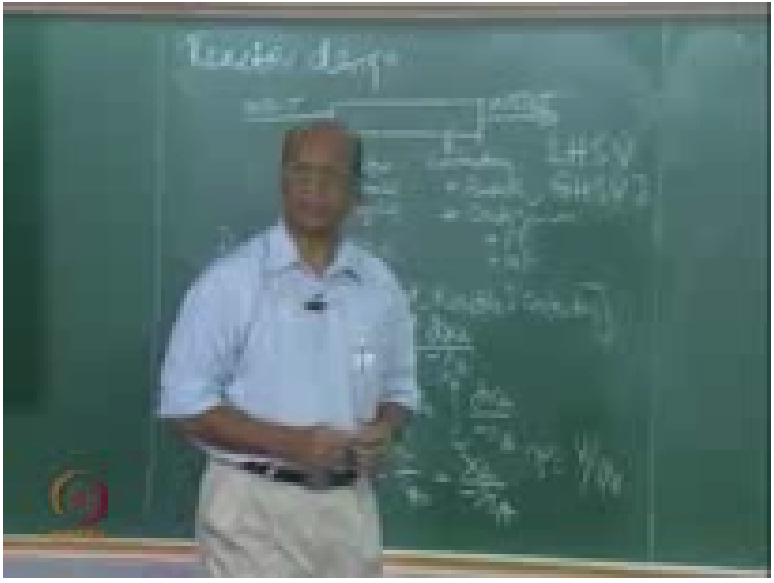
(Refer Slide Time: 56:16)



Ok where tau equal to, I write here, where tau equal to V by V naught where V naught is normally expressed only, at the entrance, Ok good.

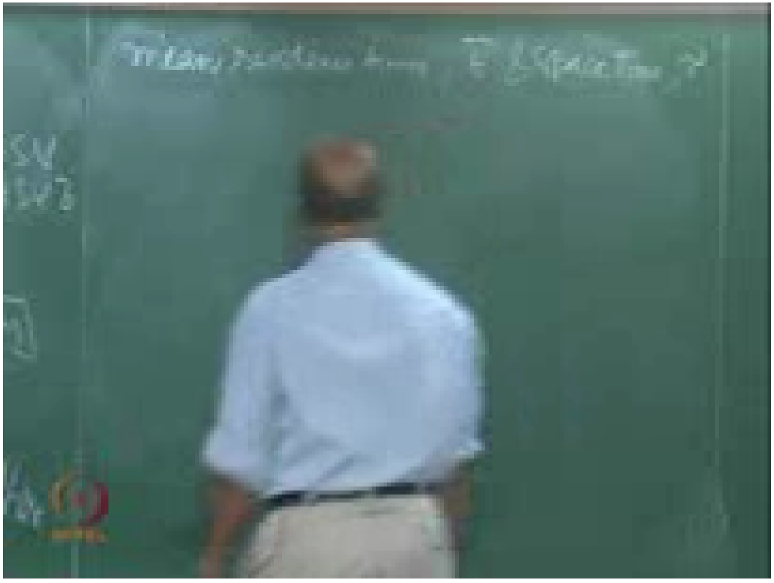
So how do you find out t bar?

(Refer Slide Time: 56:32)



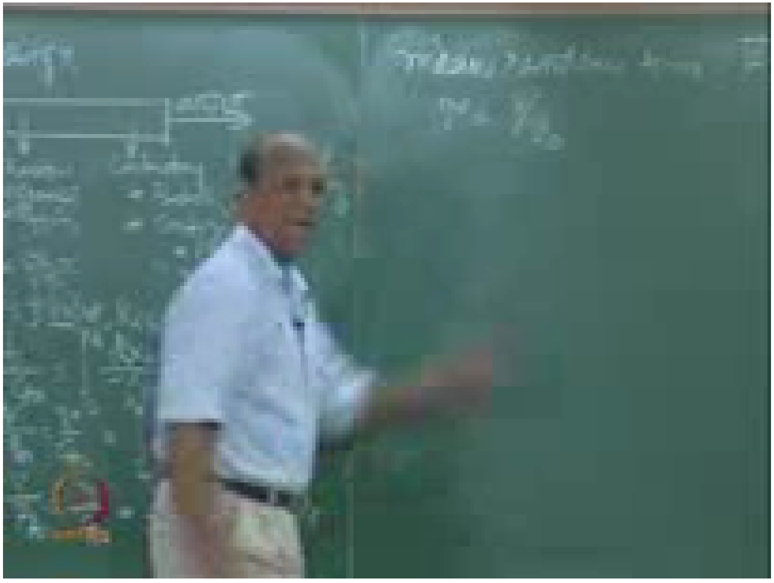
t bar is the actual flow, I mean this is very easy for imagining for packed bed, mean residence time, Oh I have to cover many things, mean residence time t bar, this one we called space time tau,

(Refer Slide Time: 56:59)



Ok. So tau is very easy to define. V by V naught and

(Refer Slide Time: 57:03)



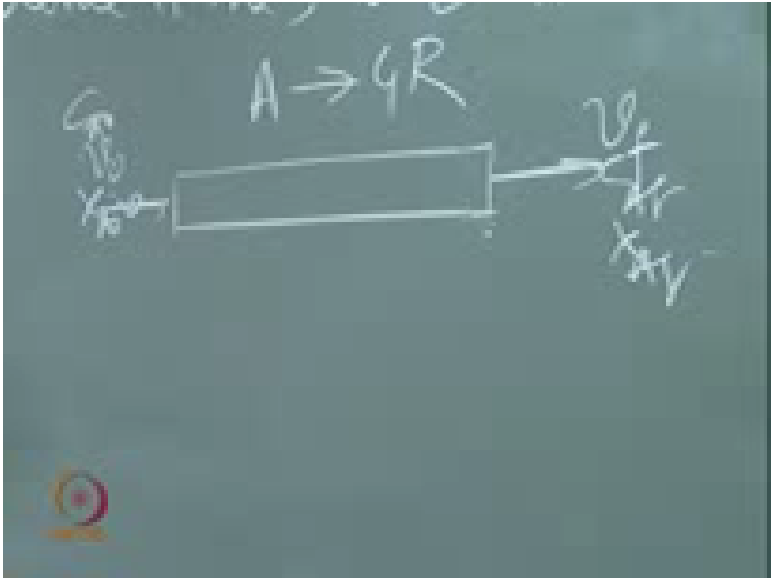
the actual definition is, words if you want to tell, that is time required for processing one volume of the reactor.

Ok. Space velocity is inverse of that where you write, per unit time how many volumes you can do that, Ok. That is the space time, good. That is nice. So now mean residence time is normally t bar, Ok. So how do you actually find out this?

So if I have a plug flow reactor which is easy to discuss, plug flow is easy to discuss here. so then I have here, may be, I think it is entering V naught, it is coming at V f and I may have C A naught X A naught equal to zero, this is C A f, X A f all that, Ok, good.

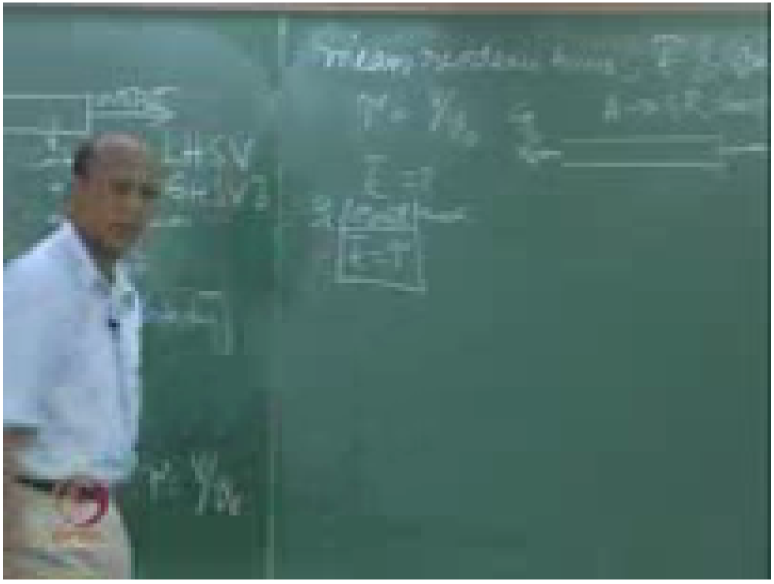
Now it is a variable volume case

(Refer Slide Time: 58:02)



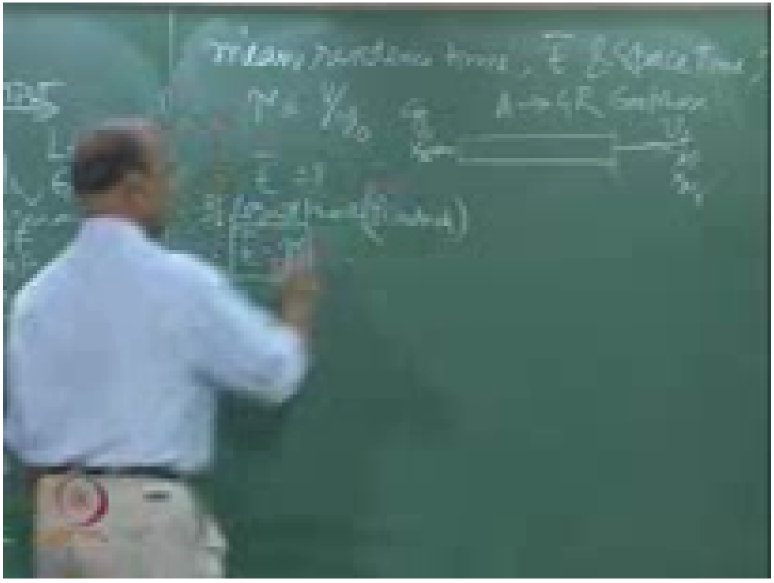
where 1 mole is going for 4 moles and it is gas phase reaction, gas phase. Ok, by the by, if it is liquid phase That I think let me also tell that. If it is liquid phase, t bar equal to tau,

(Refer Slide Time: 58:25)



or constant density system, hi funda people say that rho constant,

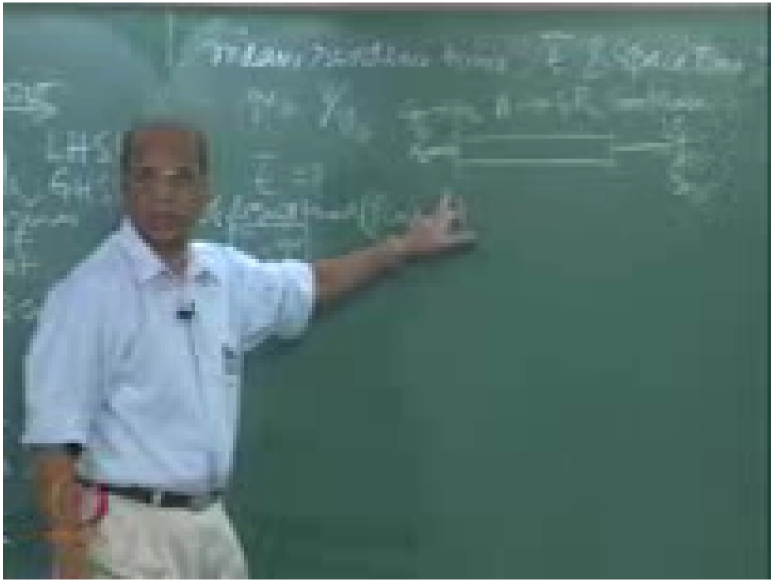
(Refer Slide Time: 58:32)



density constant, Ok good. So this is very clearly known.

Now we are talking about only variable volume, normally gas phase reactions, Ok. So if I look at the gas when it is entering, that is the phenomena that is happening and here also I have now tau equal to volume by volumetric flow rate. Because V naught is entering here,

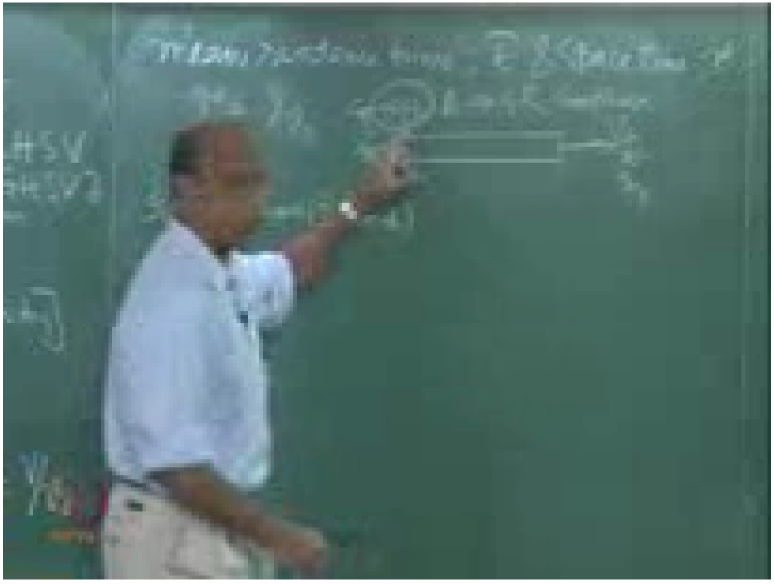
(Refer Slide Time: 58:57)



right? So I have this definition already.

But in the actual case and you know this tau is not talking anything about what is happening inside. It is not talking. As far as time is concerned, nothing is, you know stored. When say volume,

(Refer Slide Time: 59:11)



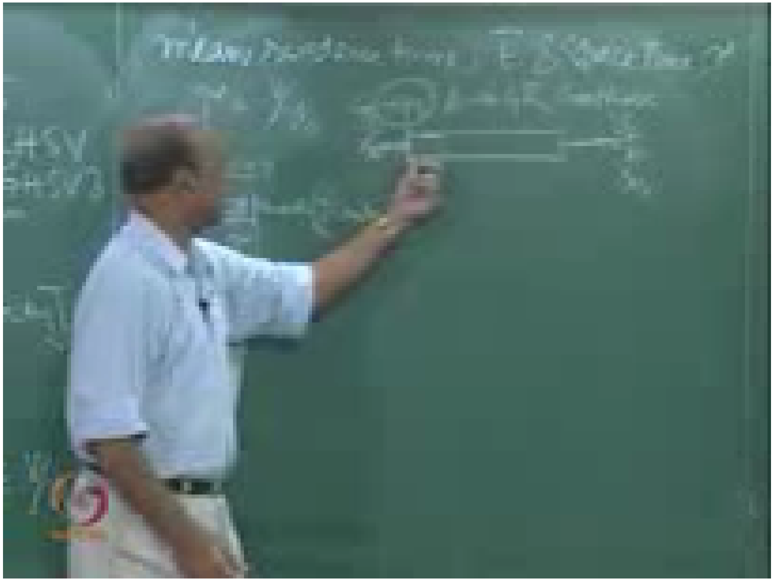
the volumetric flow rate equal to tau.

Now so even I look at this reaction A, Ok 1 mole has entered, let us say as an imagination, Ok so then it is moving from this point to this point. Let us say I have 90 percent conversion of that 1 mole, 1 mole per liter. So that means here I will have only point 1 moles per liter as far as concentration is concerned. Then how it is moving?

I have here when it comes, the moment it enters, 1 mole is going to 4 moles. Let us say there is some conversion, Ok. Let us say, I think you know 10 moles, easy for remembering, .10 moles just entered and here when I look, conversion is 10 percent. That means concentration is 9, Ok, good, so during this time what is happening to the volume?

Because conversions is Ok, moles entering and moles at that point leaving Ok divided by number of moles but during the reaction,

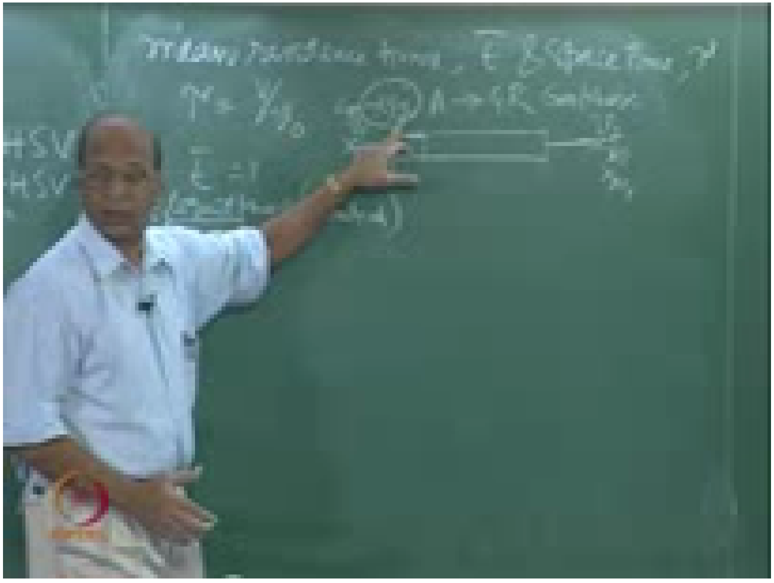
(Refer Slide Time: 01:00:11)



this one mole of A is producing 4 moles of R. It is a constant rigid pipe. So when volume of the gas increasing, what should happen to the gas molecules now?

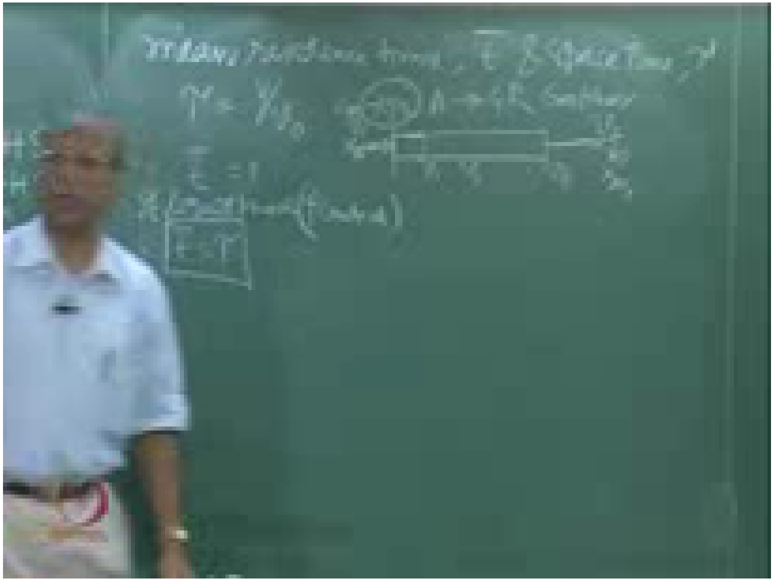
Yeah, it has to accelerate. The velocity will increase. Right, so when it is increasing with the velocity, then it moves faster. Now, our volumetric flow rate V naught,

(Refer Slide Time: 01:00:37)



is it same here? No. It will change. So it will change to somewhere V, V V 1, V 2, like that finally V f,

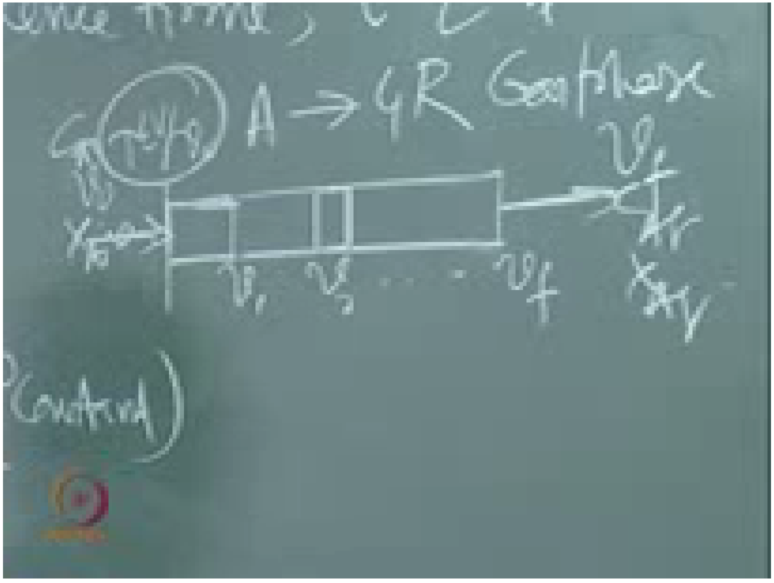
(Refer Slide Time: 01:00:48)



corresponding to 90 percent conversion whatever, right?

So now what is the, I mean how do you define t bar. t bar is the volume of the reactor, if I take a small volume here, volume element, so volume of this divided by

(Refer Slide Time: 01:01:09)

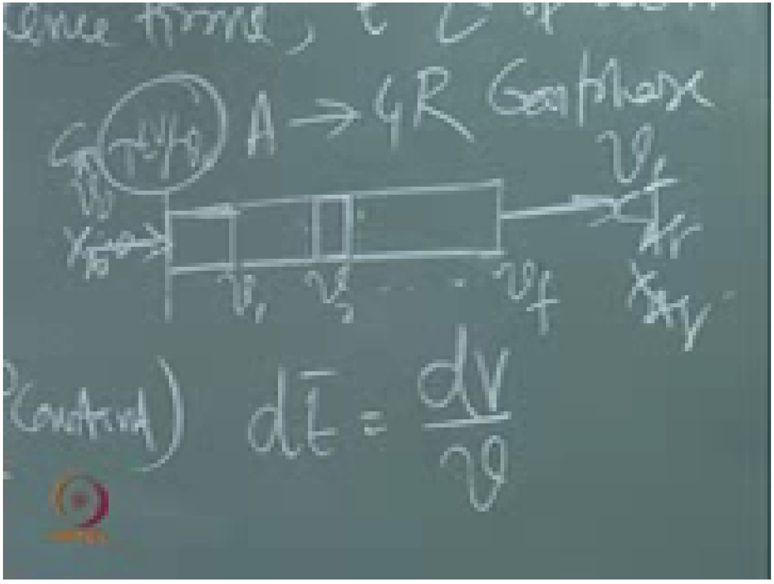


volumetric flow rate is the time, it is the time. So when that volume is increasing, then it moves much faster. Because this is not constant.

Because 1 mole is going to 4 moles, this will expand a little bit. When it is expanding a little bit, cross-sectional area is constant. So then what should happen? Length should be more, that means it will appear in terms of velocity faster, right?

So that is why the basic definition, if I take small d t bar is d V by V,

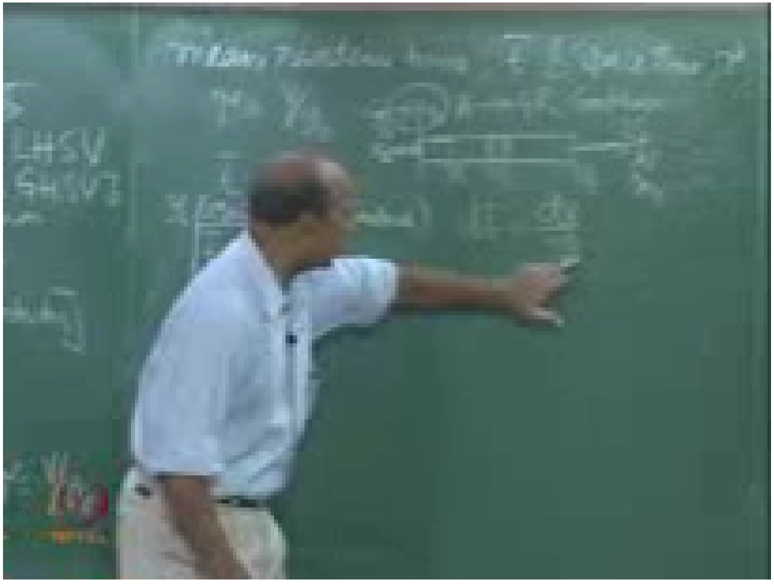
(Refer Slide Time: 01:01:46)



Ok. Now, this is not uniformly, linearly expanding. Why? That depends on the kinetics. If it is second order, it is different. If it is first order it is different. If it is third order it is different. In between any order it will be different.

So that is why t bar depends on the kinetics whereas here tau depends on only volume of the reactor divided by entry volumetric flow rate. Entry volumetric flow rate, that is all. We are not taking the volumetric flow rate inside. Whereas I am taking

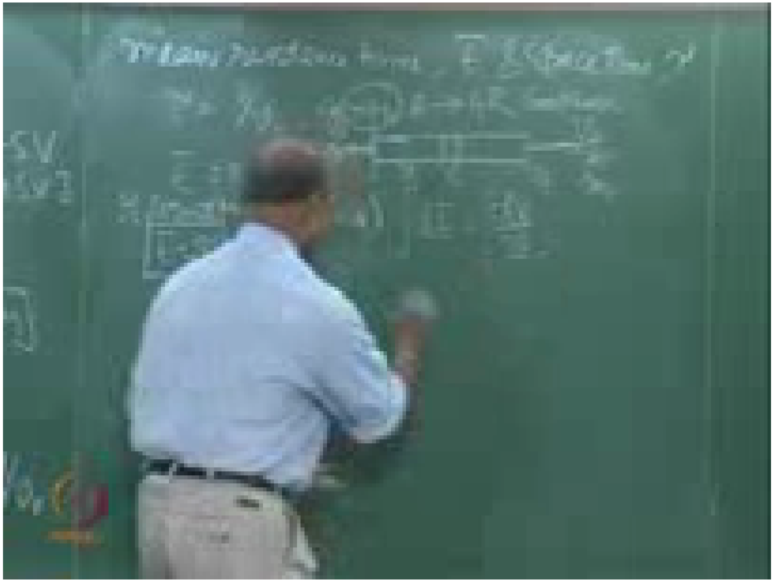
(Refer Slide Time: 01:02:22)



this volumetric flow rate inside. This is changing throughout. And this change I now have to find out.

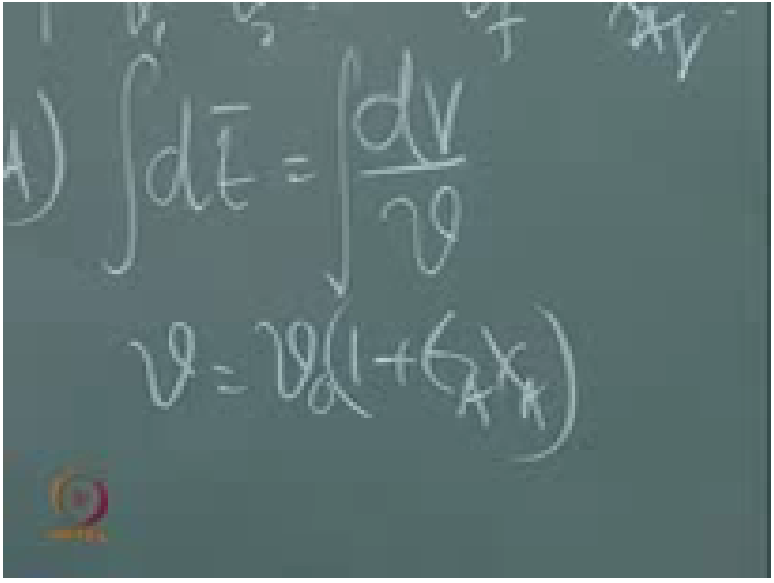
So I will now try to find out integral of this and here the volumetric flow rate

(Refer Slide Time: 01:02:38)



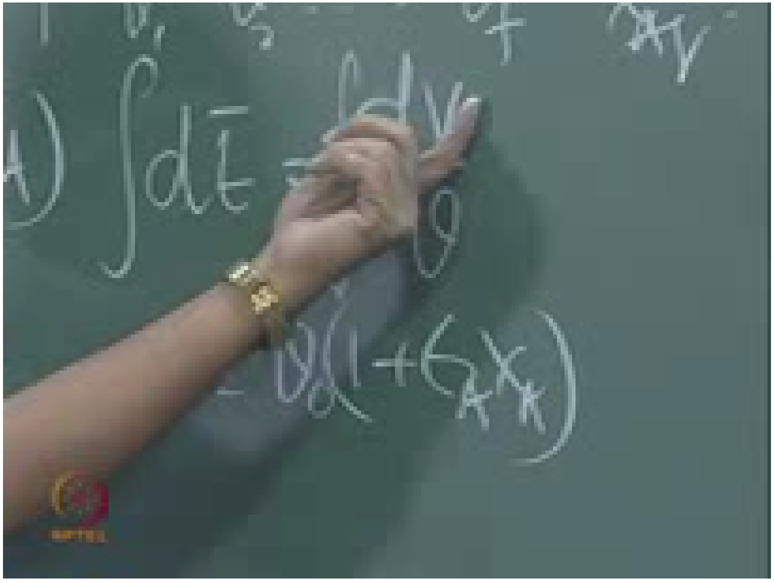
can also be imagined as same for isothermal and constant pressure system. V equal to V naught epsilon A, Ok for ideal gases. Here also we are assuming volumetric flow rate

(Refer Slide Time: 01:02:57)



also per unit time, Ok how it is changing. So that is why I have to substitute this V here and what is this d V?

(Refer Slide Time: 01:03:06)



(Professor – student conversation starts)

Student: 1:03:07.8

Professor: Change in the volume. Do I have an expression for change in the volume here? Recall your memory. The first derivation of plug flow. What is the basic differential equation for plug flow? F A naught d X A

(Refer Slide Time: 01:03:17)

equal to

Student: 1:03:22.0

Professor: Actually this d V

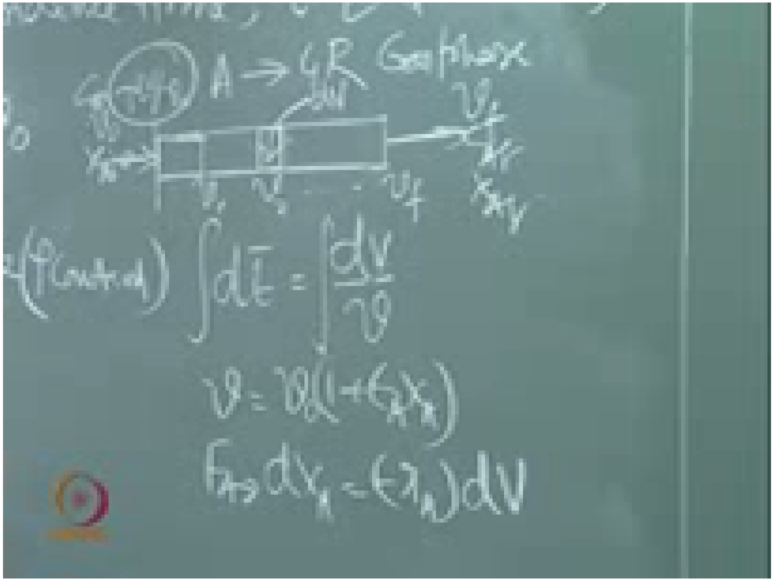
Student: V naught A

Professor: You see, F A naught d X A equal to

Student: minus r A d V

Professor: You see how much time you are taking to tell this. It is the basic design differential equation for plug flow. And we have only one plug flow, nothing else.

(Refer Slide Time: 01:03:44)

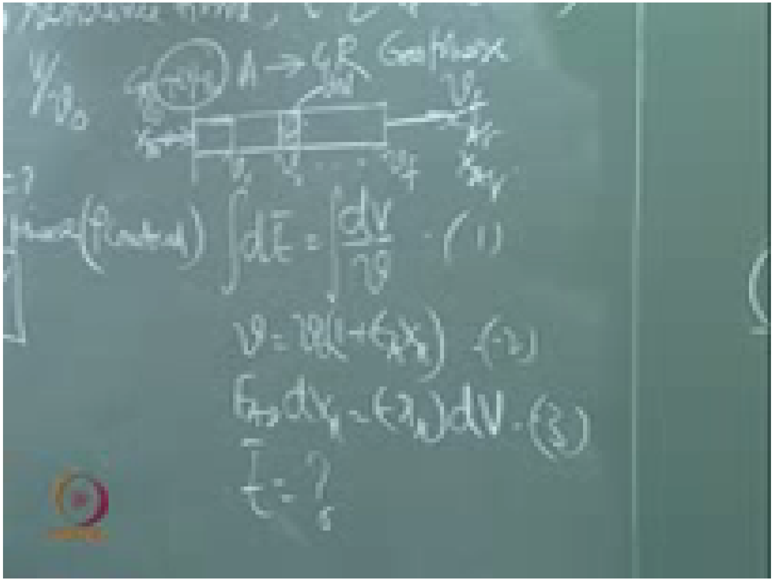


(Professor – student conversation ends)

Ok that means no practice. Absolutely no practice. Ok we do not worry about whether plug flow is increasing volume, decreasing volume, all that you do not. That is a problem.

So now using this equation, this equation, this equation, calculate t bar. I am not telling that. I do not tell you that. I gave the clue. In fact, in no other class I gave even this definition.

(Refer Slide Time: 01:04:14)



Always I will welcome them with a surprise test, all zeroes, very easy for me to correct, Ok, all zero, not even 1, right, yeah, so then I will explain in the class why you got zeroes. This is how you have to do.

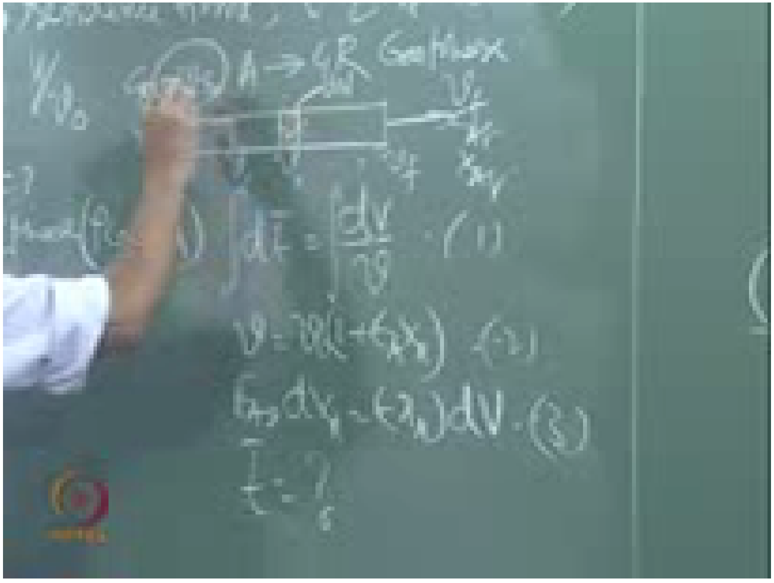
But now I gave you these clues, now you do it. But if you are only worried about all other things except C R E, again it is easy for me, all zeroes to put. You have to derive now t bar in terms of this and then see the difference between what is tau by C A naught and that t bar. Good. Very nice. That is the definition of t bar.

And you can now calculate for first order reaction, you know what is t bar, what is tau. For second order reaction, you know what is t bar, what is tau. For zero order reaction also you can calculate, order reaction, what is t bar, what is tau. Right.

So all these things, you have to make somewhere, some corner in the notes and then that, you know, this fellow is a dangerous fellow, he may give this one in the examination. And all that you have to write and then you have to prepare for that. Not 1 day before, now itself. Ok, good, excellent.

So this is again now t bar, tau is it clear? Remember this figure, this volume

(Refer Slide Time: 01:05:32)



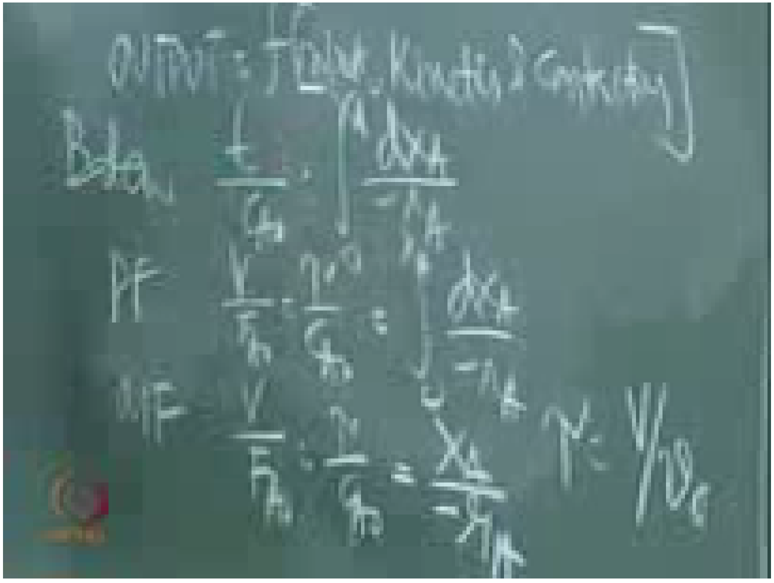
when it is entering, it is different. You know it expands a little bit, then expands, then expands, then expands. That expansion depends on whether you have first order reaction, second order reaction, and whether number of moles, whether 1 going to 4, or 1 going to 2, or 1 going to 100. Ok. 100 may not be there but I think large values. So all that will come into picture.

Because use that, the moment you say, someone says t bar, your mind should go to that volume. That volume is no more constant. It is moving, different speeds at different location. Average of all that speed is called t bar, mean residence time. That is the thing. That is the funda, right, average of all that.

Because it is not uniform. If it is linear throughout, then I think you know we know how to easily find out. It is not linear. Some case it may be linear, some case it need not be linear, Ok. The time changes depending on the, volume expands and depending on the volume expansion time of these molecules change inside the reactor, Ok, good. So t bar and tau also now it is clear for you.

So next one is, yeah the reactor design expressions also I have given now, good. So now using these equations, how do you calculate actual design expressions? Integral expressions. These three I have. Example, if I have batch reactor as

(Refer Slide Time: 01:06:56)



OUTPUT = f[Input, Kinetics & Contacting]

Batch $\frac{t}{C_{A0}} = \int \frac{dX_A}{-r_A}$

PF $\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \int \frac{dX_A}{-r_A}$

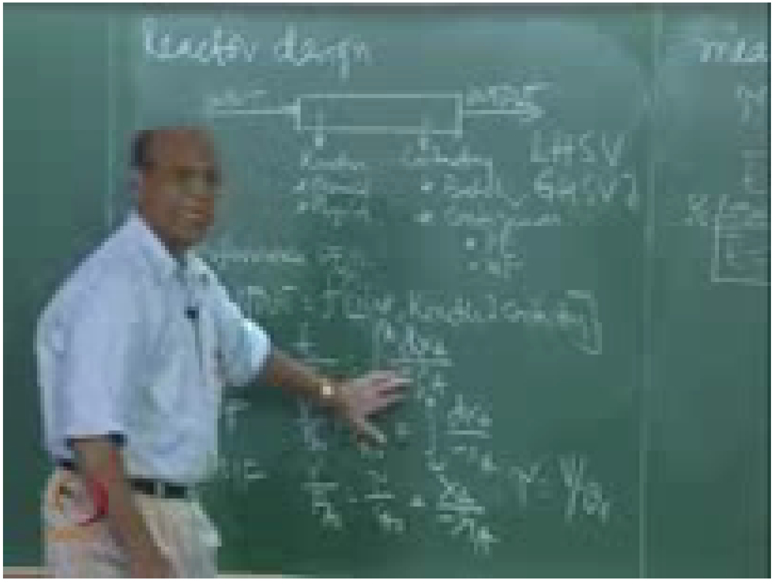
MF $\frac{V}{F_{A0}} = \frac{\tau}{C_{A0}} = \frac{X_A}{-r_{Af}}$ $\tau = V/v_0$

first order reaction, simple k into C A, so what is the design expression for me in terms of integral equation?

This is the one which you have to integrate but minus r A is a general one. So finally when you are actually calculating this time, that time depends on this kinetics which is first order, second order, reversible first order, reversible second order, the reversible second order one what you have done in the, yeah in that assignment, you know to find out the volume, Abdul, yeah.

So but you know if integration is difficult then what do you go for? Numerical. If numerical also may not be giving you exact answer what is the best one, graphical. Area under the curve. But you should know how to count area under the curve. If you do not know, then it is a problem. So that is why I can also give you just one or two equations, for example batch reactor

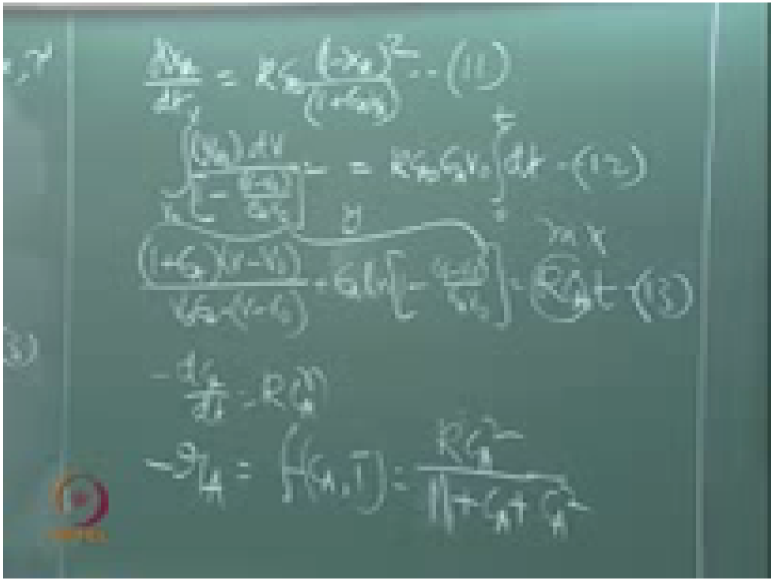
(Refer Slide Time: 01:07:47)



is Ok, we have done for first order, second order and all that, Ok. And variable volume also we have done. These are all batch.

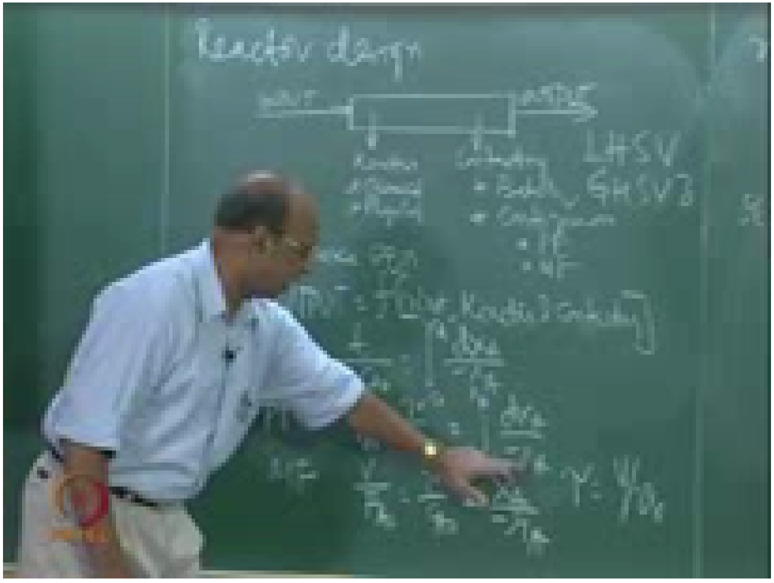
So that is why I will give you some

(Refer Slide Time: 01:07:57)



equations for plug flow and mixed flow, variable volumes. Because constant density is very easy, right. But all the time what you have to do is, you have to only use these two expressions, V by F A naught, d X A by minus r A,

(Refer Slide Time: 01:08:16)



substitute here for minus r A, k into C A, do not try to integrate automatically without converting into X A.

Ok, because there may be people who do not know that X A, C A different. Simply they may use it. Right. That is why you have to convert this into the....otherwise you also have other possibility of using this equation in terms of concentration. But that is a special case, special case like what, Swamy?

(Refer Slide Time: 01:08:44)

(Professor – student conversation starts)

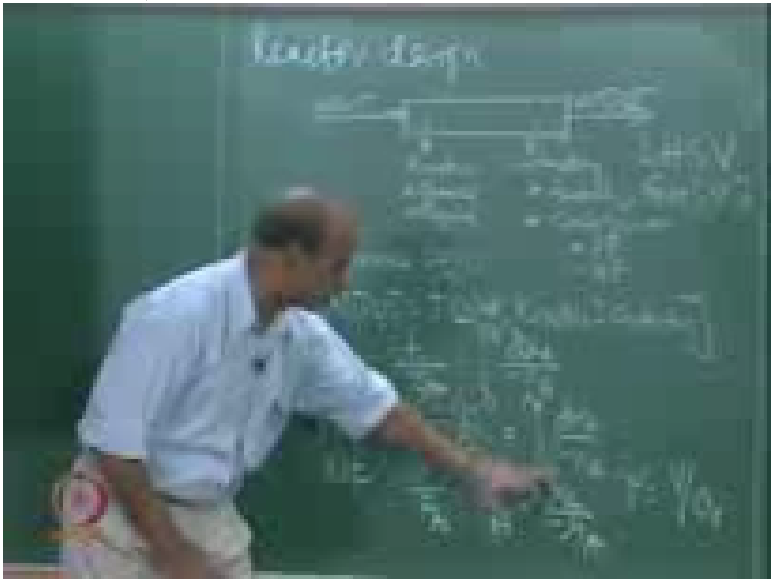
Student: Data which is having less concentration

Professor: You can convert one from the other, that is not a difficulty. That is not the one. Abdul, when do you use C A, when do you use X A?

Student: Constant density system

Professor: Yeah, if it is a constant density system, because many people may have doubt, why this fellow always writing in terms of X A and in earlier course, B Tech we also wrote in terms of C A? Ok. You may have that doubt. So the answer for that is X A is a general expression. Whether volume change or no volume change that can be used. But C A if I write it is restricted. Only for constant density system. That is the reason why people use this kind of X A equations. Repeat

(Refer Slide Time: 01:09:02)



(Refer Slide Time: 01:09:29)

Why do I use X A, why people use X A all the time?

Student: X A is a general expression

Professor: Very good, yeah.

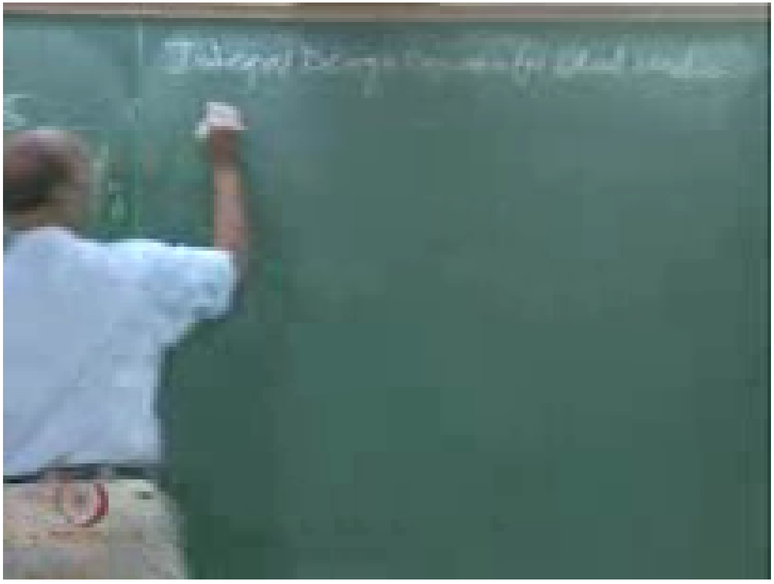
Student: If you use C A that is a constant density system.

Professor: Yeah, that is a specific case. So now that is the one.

(Professor – student conversation ends)

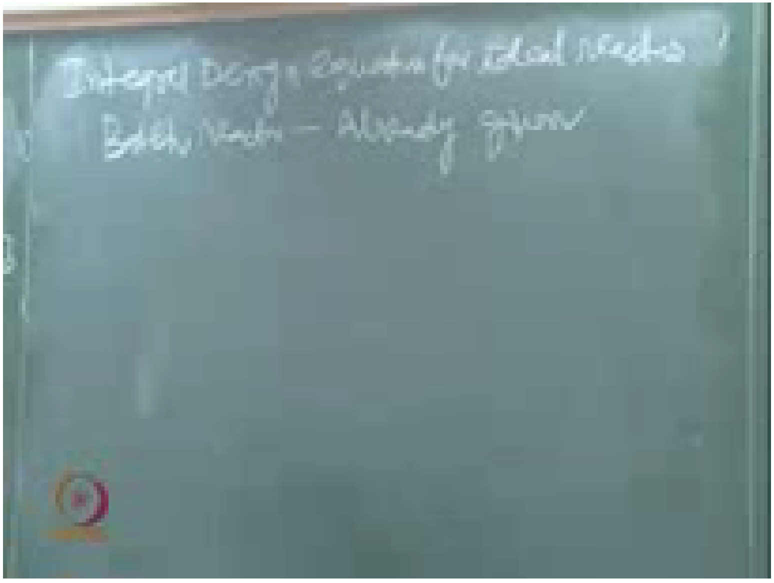
That is why we use only these equations and I will give you integral design expressions, design equations for ideal reactors, Ok,

(Refer Slide Time: 01:10:02)



batch reactor already given, (laugh) you may not know, I say. You may not know, I say. So that is why,

(Refer Slide Time: 01:10:17)



Integral Design Equation (for ideal reactors)
Batch reactor – Already given

because you will search.

Because when I ask you what is the basic differential equation for plug flow, no one could say no, they went again, flip flap sound I have heard , so going to the old papers and then only trying to tell that. That equation also you cannot forget. F A naught d X A equal to minus r A into d V. What is for mixed flow reactor?

(Professor – student conversation starts)
Student: minus r A
Professor: minus r A into, yeah F A naught into X A equal to minus r A into
Student: V
Professor: V. Is it difficult to really remember that? So easy. Even for batch also you can write that differential equation first. Ok, good.
(Professor – student conversation ends)

So then you have plug flow reactor, first order, zeroth order I do not write, First order, first order reaction. So now there are so many cases here, A going to 4 R, gas phase. Because you know I am a very tricky fellow. My question papers will be very good. Ok.

I will give R going to, sorry A going to 4 R, but somewhere I will write it is liquid phase reaction. Ok, but immediately you feel that Oh, A going to 4 R, volume change so let us now take epsilon and all that. You will get zero mark. Ok that is why be careful. Read properly, right?

So A going to 4 R is not automatically gas phase reaction,

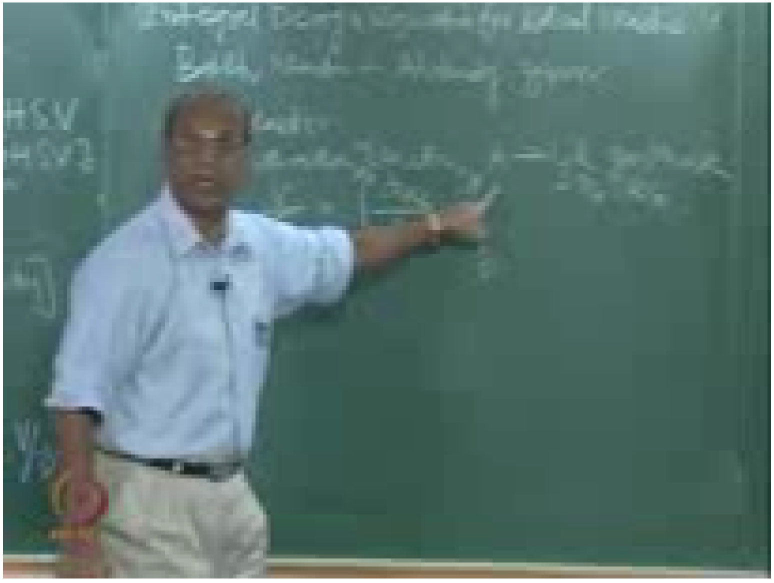
(Refer Slide Time: 01:11:48)

right. It can be also liquid phase reaction. That is why I have to give. If I do not give, you scold me. Like I am scolding you, you can also scold me, no problem. Ok good.

So this is gas phase reaction. What is the equation what you get? So design expressions we have talking. V by F A naught equal to integral zero to X A d X A minus r A so this is, Ok, this first order reaction I told no, minus r A equal to k into C A, Ok.

Here also I have to write it is elementary reaction.

(Refer Slide Time: 01:12:25)



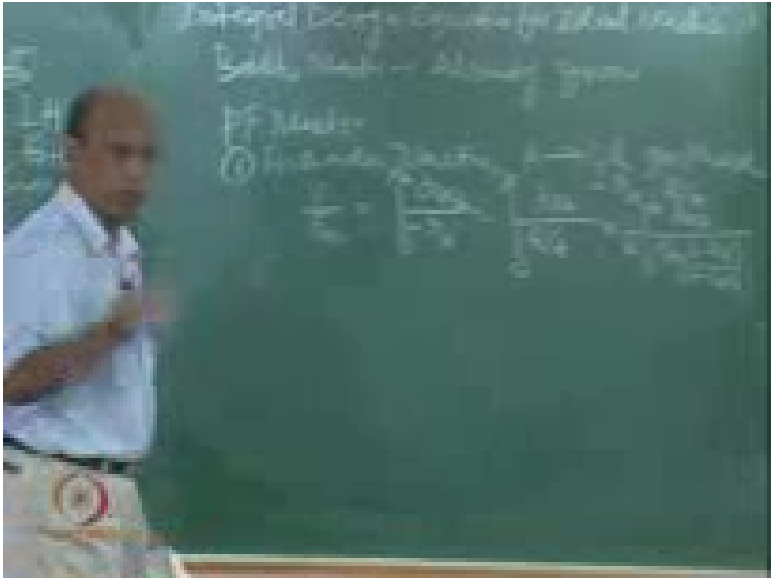
Otherwise you do not know what to write, right. If it is elementary only it is first order. If I say it is non-elementary then you give me the rate equation Sir, you have to ask me. Good.

So this is equal to d X A by k C A again which is equal to zero to X A d X A by, k I can bring out, yeah this is C A naught, yeah C A naught that also I can bring out but let me write first time, epsilon A X A. This is what you have to now integrate, right? Yeah.

And again I have not told this one is pure gas or impure gas, right? If I say that this is only 50, 50 percent inerts and all that, then epsilon will change. Otherwise you have to take pure gas means, so all these statements must be given there.

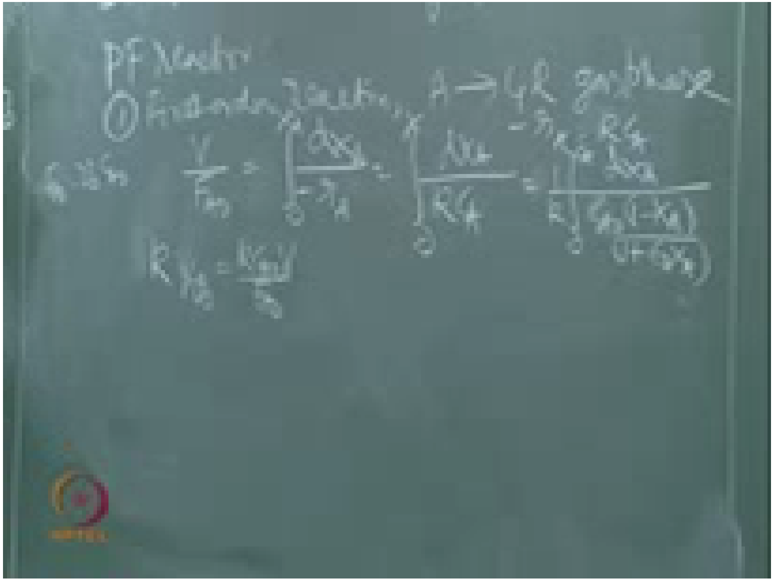
So the equation what you get for this, for easy one I am taking k tau, tau equal to volume by volumetric flow rate,

(Refer Slide Time: 01:13:27)



so this design expression, Ok, k V by V naught, so in terms of F A naught what is that come, or F A naught equal to V naught into C A naught. So when I write that also, V naught if I write, F A naught by C A naught, Ok, so this is also equal to, please check me. k C A naught by F A naught, correct, is it right? So many subroutines

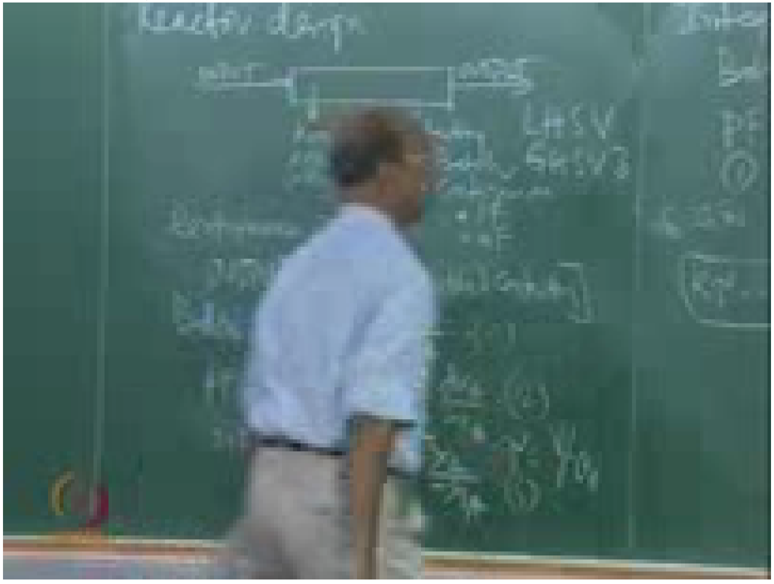
(Refer Slide Time: 01:14:00)



inside, Ok so this is the equation. Yeah.

This is the reason why I was telling sometimes tau we use because simple to write. Instead of this equation, this equation is simple. Ok, yeah, now this is equal to, this you have to derive, minus, yeah 1 plus epsilon A l n 1 minus X A Ok, minus epsilon A X A, anyone remembered this during their B Tech class? Now I have to go to 1, 2, 3

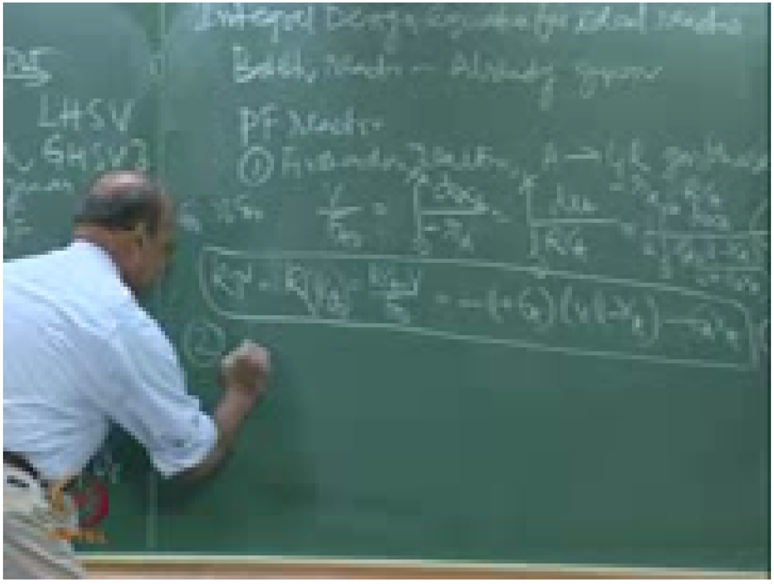
(Refer Slide Time: 01:14:46)



all this is 4, this is 5.

So I just gave this example because this is slightly more complicated to write. So that is why k tau is easiest one, right? That is the reason. If it is second order, second is,

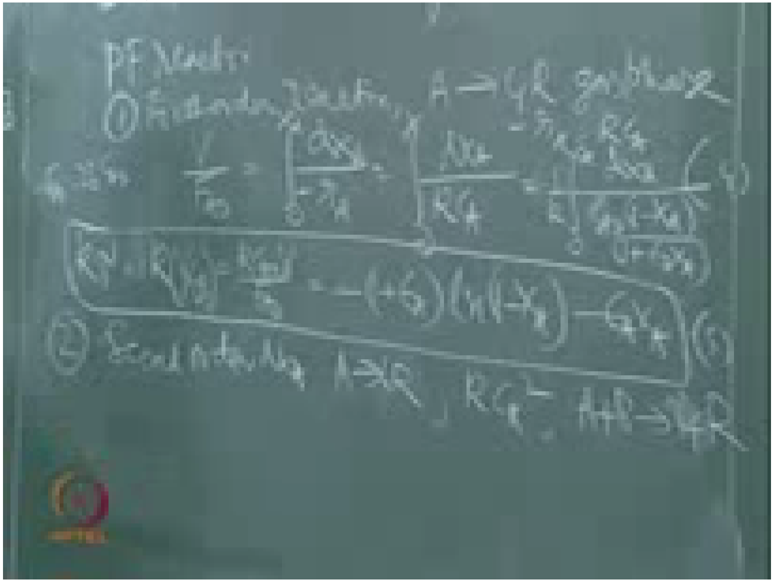
(Refer Slide Time: 01:15:06)



first order, second order, this is simple A going to R k C A square, or maybe A going to 4 R also I can take. So there is volume change. May be this is 4 R, right? You know there are so many cases.

This can be A going to 4 R or the other one may be A plus B, this k C A square, A plus B going to products again, Ok some change, again 4 R,

(Refer Slide Time: 01:15:43)

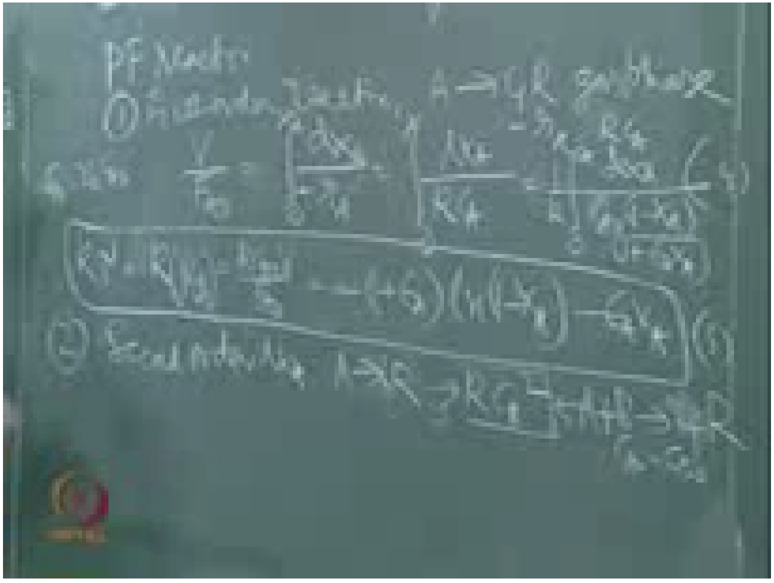


right but C A naught equal to C B naught. I will get again same equation only. You see so many conditions. That is why reaction engineering is hell. Because one small thing changes, entire equation changes, Ok.

So otherwise the moment I change, this C A naught is not equal to C B naught, then you have again complicated equation, that means it is not 1 mole, 1 mole, initially. It is 1 mole and 3 moles. C B naught is 3, and C A naught equal to 1, then again you have the problem.

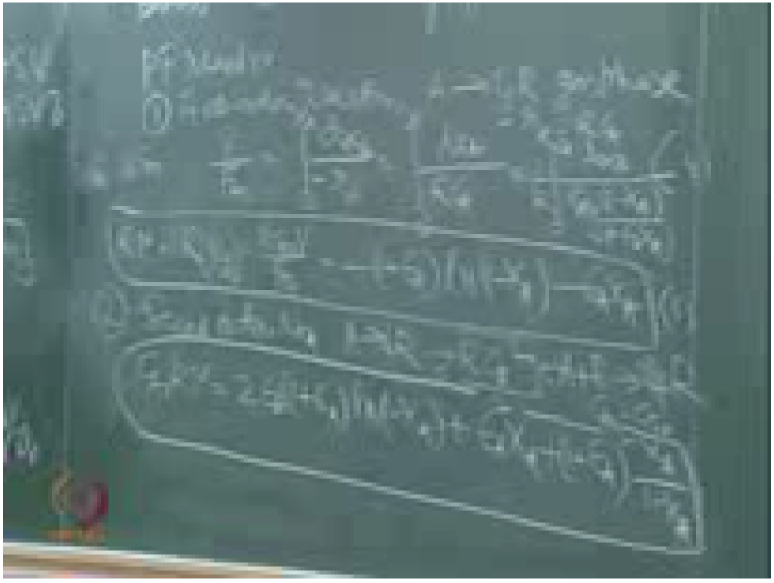
So that is why in these 2 cases it is same equation. That means C A naught equal to C B naught, so many conditions. So the equation what you get here is

(Refer Slide Time: 01:16:25)



C A naught k tau equal to 2 epsilon A 1 plus epsilon A l n 1 minus X A plus epsilon A, epsilon A square X A plus 1 plus epsilon A square X A by 1 minus X A. This is the equation. Yeah.

(Refer Slide Time: 01:17:09)



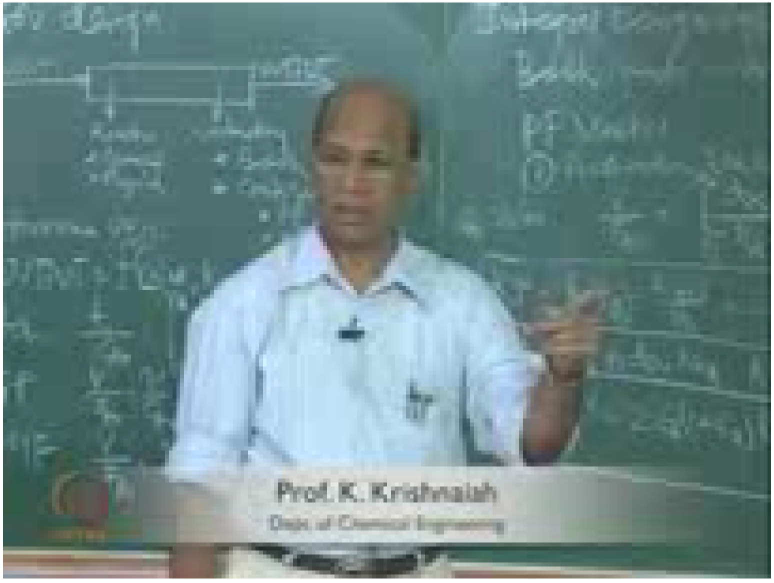
Just to give you, you know some kind of taste for you and this is what you have to derive in the examination if I ask you second order with volume change, Ok. You can simply; this is a general expression. You can simplify when epsilon equal to zero. Tell me, when epsilon equal to zero, what do you get from this equation?

(Professor – student conversation starts)

Student: X A by minus 1:17:32.8

Professor: Good, that is what for constant density system what you remember which is also same for which reactor?

(Refer Slide Time: 01:17:39)



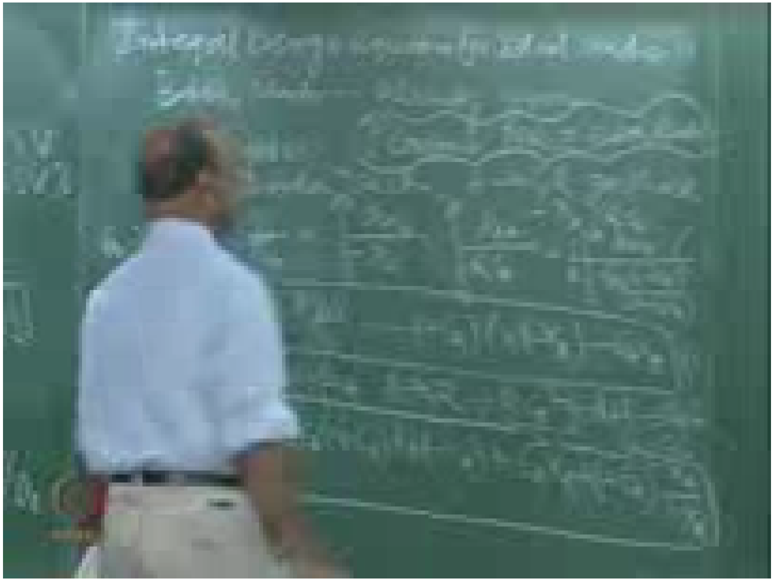
Student: Batch

Professor: Batch reactor, batch reactor also you get.

(Professor – student conversation ends)

So all constant densities, yeah, this also you make a note somewhere. All constant density systems, batch reactor and plug flow reactor same equations, rho constant P F R equations are identical to batch, batch reactor, yeah.

(Refer Slide Time: 01:18:09)

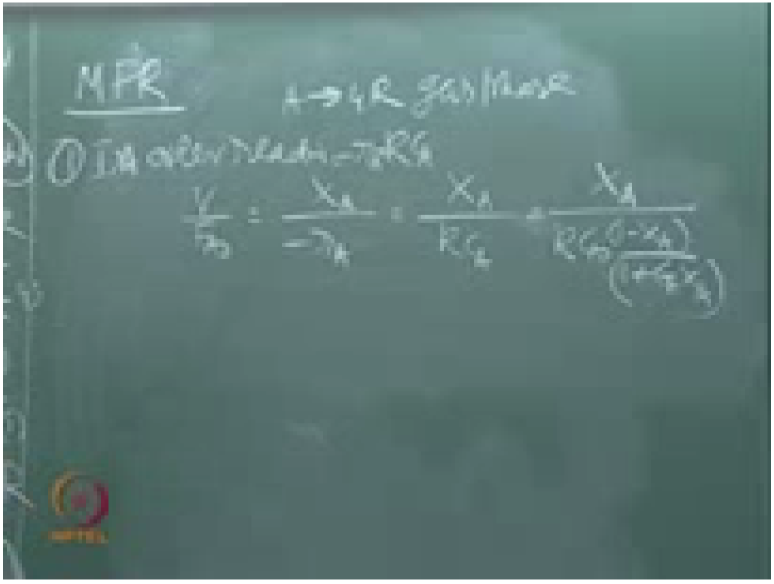


Ok.

So I think in Levenspiel book many integral equations are given. You have to derive them. Do not blame me at that time, Ok. So unless you derive on your own, definitely you won't understand all that, right. And the mixed flow reactor is very nice guy. Mixed flow reactor, why it is very nice guy? There is no integral there.

Ok, so if it is first order reaction, let us say k C A square, sorry, first order reaction minus r A equal to k C A, maybe I also have A going to 4 R, gas phase reaction, what is the equation? V by F A naught equal to X A by minus r A where minus r A is written as X A by k C A square, sorry, by k C A which is also equal to X A by k C A naught 1 minus X A by... 1 plus

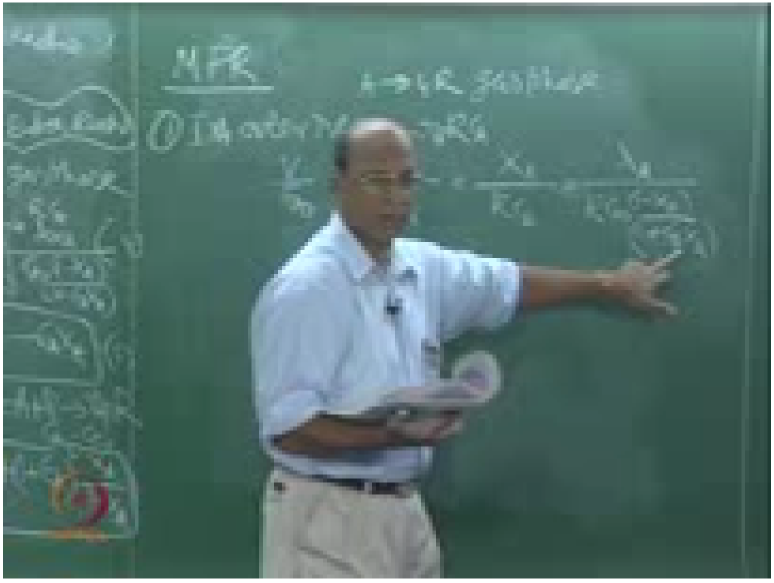
(Refer Slide Time: 01:19:33)



X A, right?

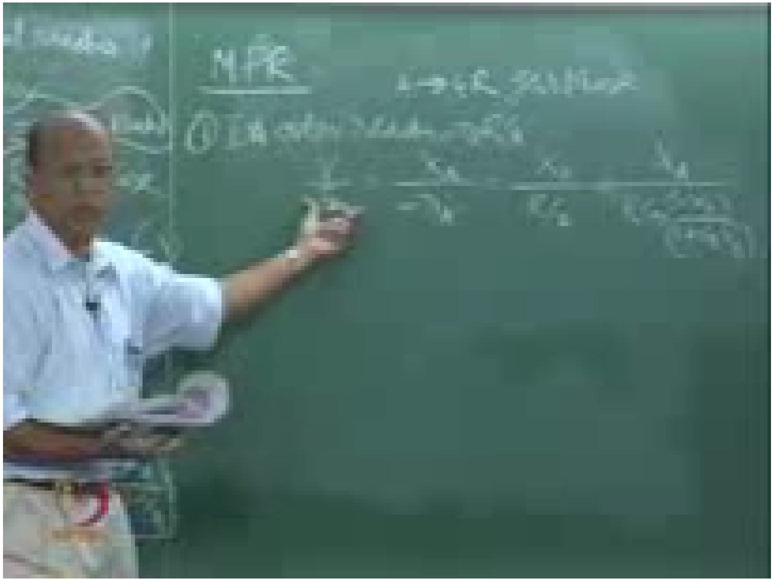
So like that for second order also, now I will have C A square, then I will have here C A naught square, all these, whole square. So like that it is very easy because it is not integral expression. It is simple algebraic expression and if I ask you what is the volume, what is the volume for 90 percent conversion, epsilon you will know,

(Refer Slide Time: 01:19:56)



because I have to give either pure or impure and epsilon you will know, X A 90 percent, C A naught definitely you should know in the beginning you are sending, then k from kinetics, right and you can directly calculate, F A naught is known to you,

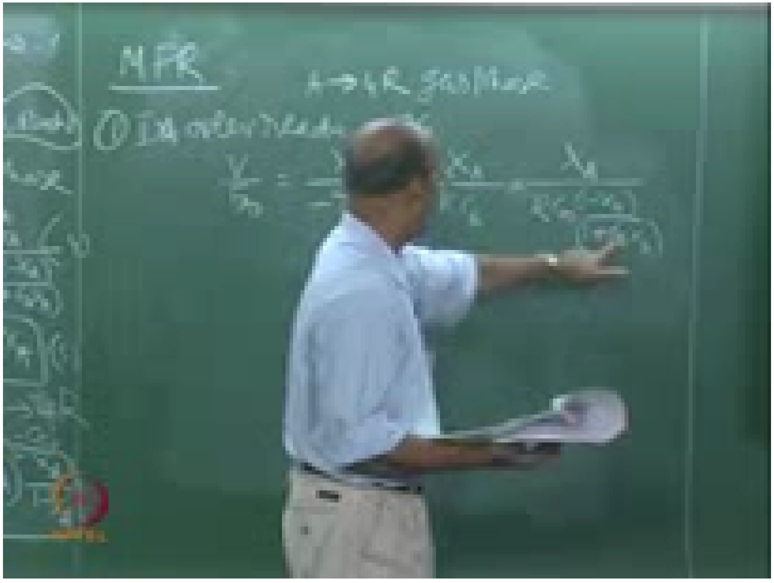
(Refer Slide Time: 01:20:11)



and V can be calculated.

That is what is that performance equation. V for given X 90 percent, epsilon equal to 3 in this case

(Refer Slide Time: 01:20:20)

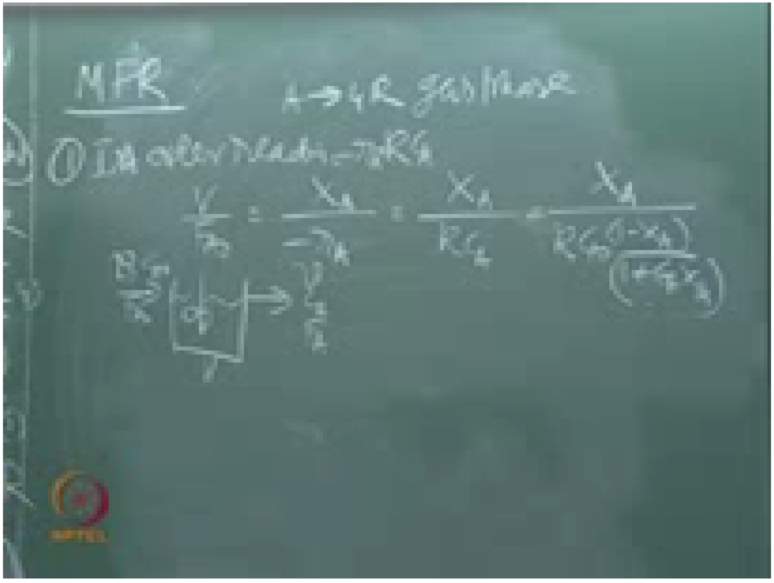


and C A naught equal to some 10 moles per liter, then k equal to 1, all that you substitute and get V, right? Yeah. So F A naught is the input and kinetics k and C A, you know this first order will give me , this k into C A is from kinetics and this entire equation is from contacting, right, very good.

So this is how you have to develop the equations and this is very easy for us, particularly mixed flow reactor and for mixed flow reactor there is another way of writing the material balance. Here you got, you know F A entering, F A naught entering, F A leaving and what is reaction under steady state conditions what we have done.

But sometimes we also write for mixed flow, this is also, let me tell you, this is very convenient way of writing, yeah here I have V, most of the time it is liquid phase reaction,Ok, C A naught F A naught, V C A F A this is volume V, right.

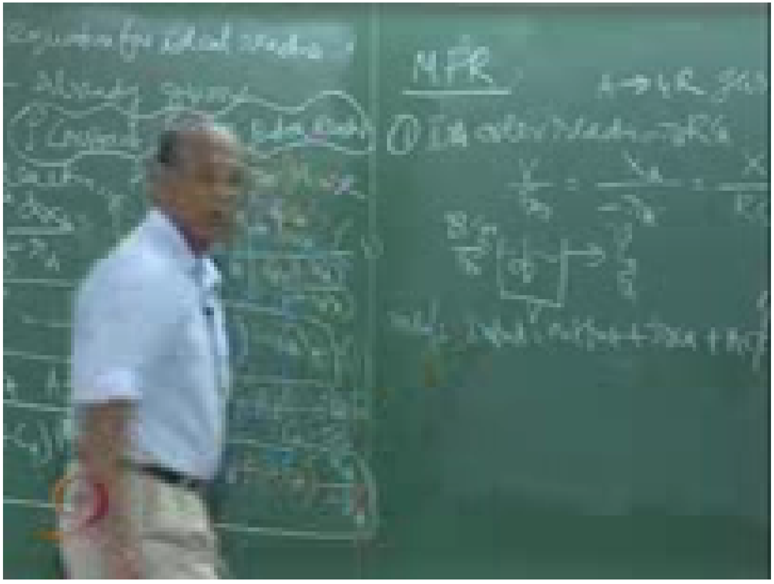
(Refer Slide Time: 01:21:27)



So one way of writing the material balance is what is entering, input equal to output plus reaction plus accumulation, this fellow is zero. We do not like accumulation, steady state people, Ok good.

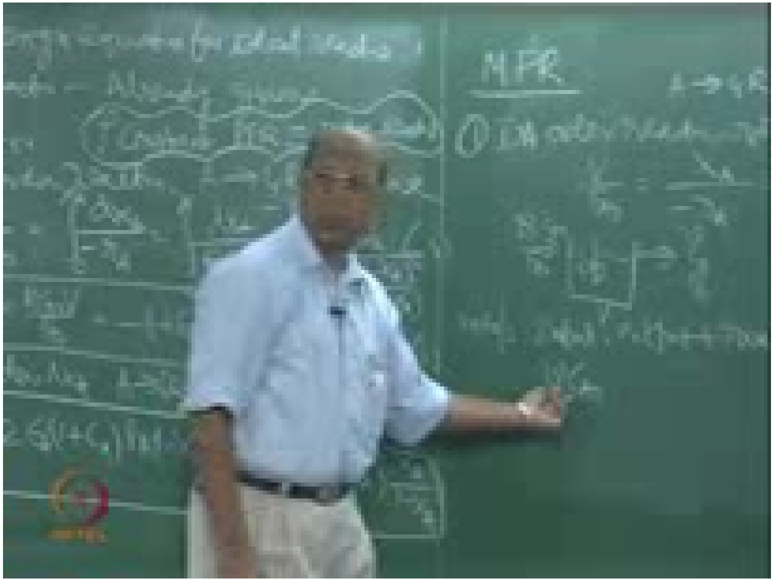
So input is, what is this actually writing? moles per

(Refer Slide Time: 01:21:50)



moles per time, so this I can write as V C A naught, what are the V units, Pooja,

(Refer Slide Time: 01:21:57)



and what are the units of this?

(Professor – student conversation starts)

Student: Moles per meter cube

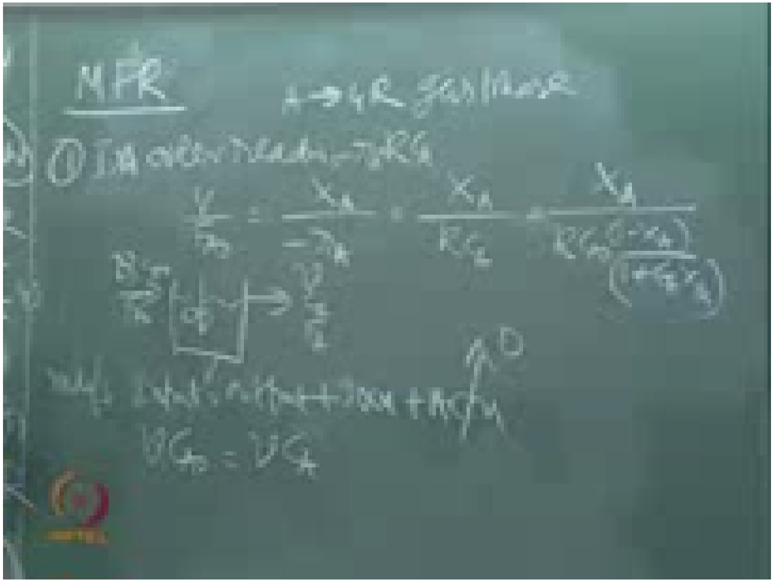
Professor: So meter cubed, meter cubed will get cancelled, you will get moles per

Student: Second.

Professor: Second. Ok, so then this is equal to V into C A. What is minus r A? I mean reaction?

Student: k C A

(Refer Slide Time: 01:22:15)



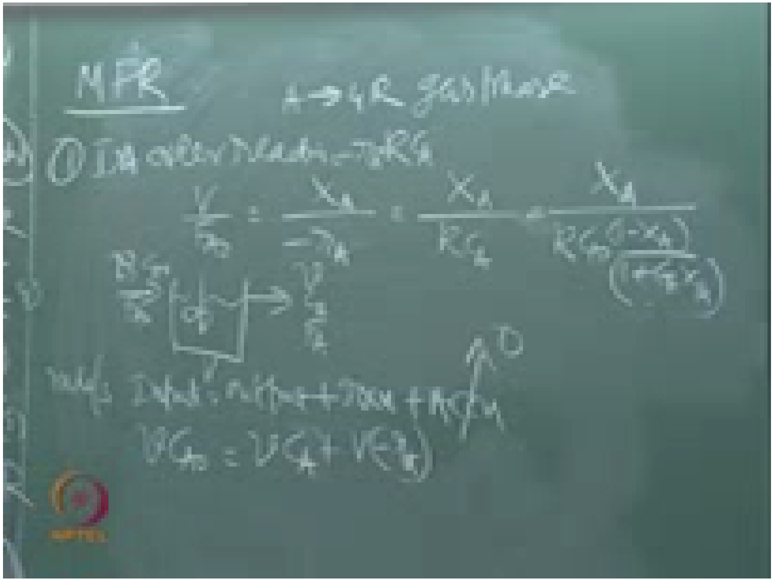
Student: First order reaction?

Professor: Yes, this is a first order reaction but in general you tell me for normal, any order?

Student: V into r A

Professor: Plus V into minus r A,

(Refer Slide Time: 01:22:28)



Ok, this also gives you simplest form, C A minus, C A naught minus C A equal to, all that you can. This is another way of writing. For liquid phase reactions, when you write this in term, no, without writing, in terms of conversion, algebra will be a little bit simpler, algebra will be simpler.

(Professor – student conversation ends)