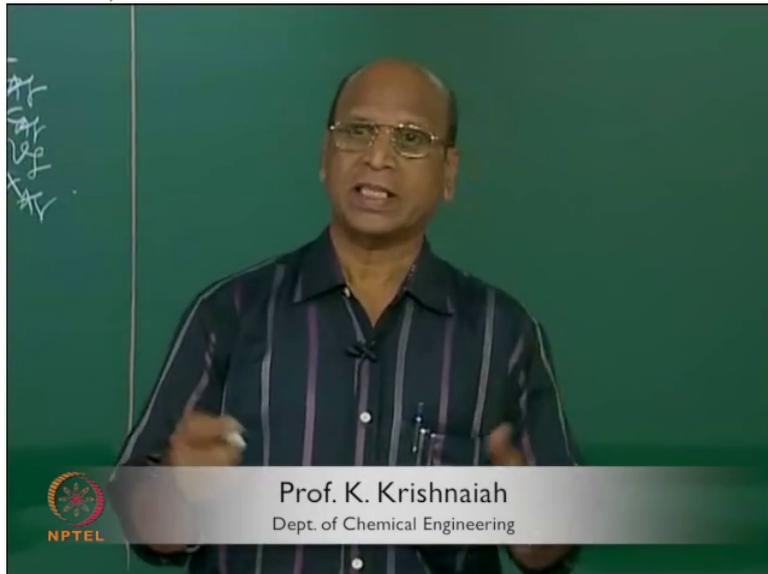


Chemical Reaction Engineering 1 (Homogeneous Reactors)
Professor R. Krishnaiah
Department of Chemical Engineering
Indian Institute of Technology Madras
Lecture No 14
Design of Plug Flow Reactors Part 1

Ok yeah, so yeah, in some cases, we would have definitely seen

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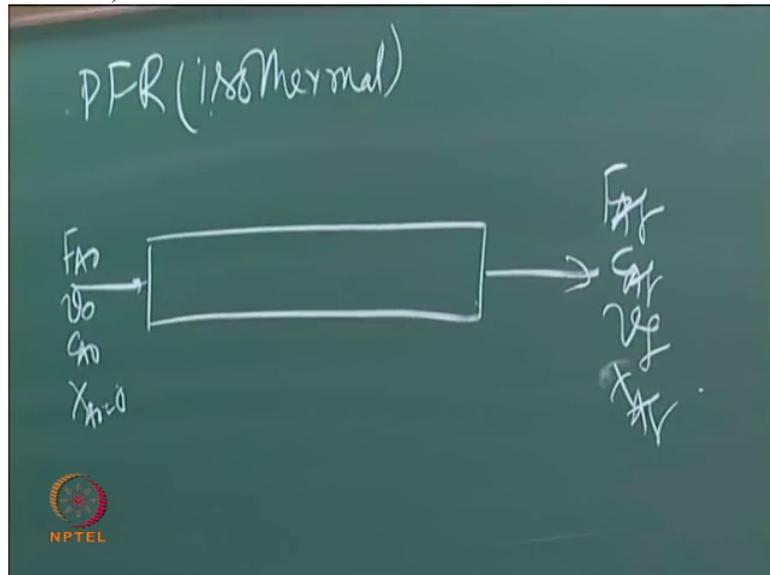


that the performance of plug flow is exactly identical with the performance of batch, Ok. Physically can you see any correlation between these two? This is a flow reactor where continuously you feed, continuously you are getting. The other one is the batch reactor, but still you will get the same, given you know the same volume, you may get the same time for the some conversion.

Here also I can calculate tau no? In this also we can calculate what is the residence time required for certain conversion and residence time is equal to volume. Correct no, volume. Residence time is equivalent to volume, right? And of course we are talking only about only reaction time.

When you talk about batch, when you are comparing plug flow and batch, you are talking about only reaction time, right. The other times you cannot take. So definitely then plug flow is better in that case because it is continuous. You do not have to discharge, you do not have to again refill, you do not have to

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again all that you know.

Once you start, you know years and years you can run the plug flow reactor all the time, Ok, good, yeah. But physically can you say that why both are giving same, under certain conditions? And to give you the clue, that condition also I will tell you. The condition is constant density system, Ok. So under constant density system why the performance is the same?

Can you imagine something? Because we have to extend your imagination, Ok. Why, because you already know that information that plug flow is also equivalent to batch under some conditions. But normally you should have a question, Oh that is a batch reactor. This is a continuous flow reactor, why same?

And mathematically if you calculate you will get the same timings or the same conversion for a given time. You get that, but did you think, a little bit of extension other than thinking that Ok this question will come in the examination so let me do somehow. Ok. Simply the, here length by velocity coordinate is replaced by; length by velocity will give you what?

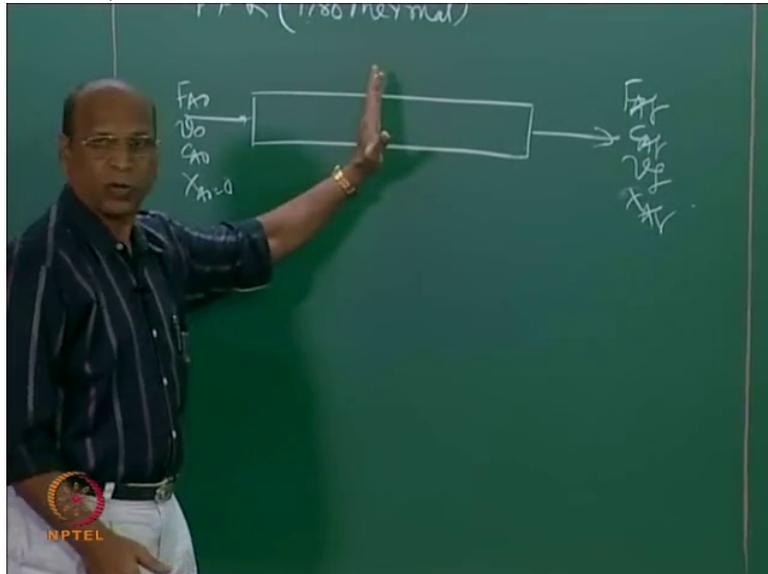
(Professor – student conversation starts)

Student: Time

Professor: Time, that time if it is just replaced in a batch reactor, batch reactor time both are exactly same. That means the time here with respect to space is equivalent to there time of

reaction. That means if 10 seconds let us say, you are here. And you have some conversion. You can find out what is

(Refer Slide Time: 02:59)



the conversion at this point. And same 10 seconds if you wait in the batch reactor if the constant density system is there, you will also get the same conversion. How do you define plug flow?

Student: Same residence time

Student: Every molecule...

Professor: Same residence time. In batch reactor what will happen?

Student: Same residence time 0:03:21.4

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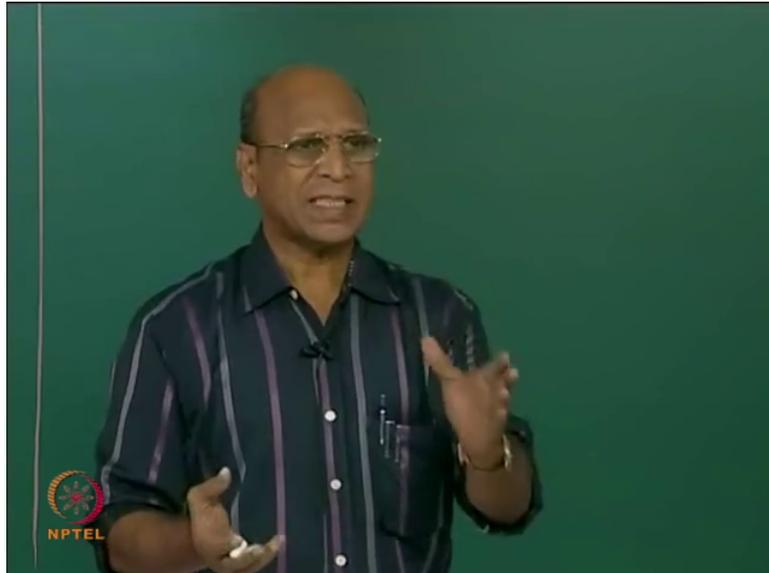


Professor: Simply concept.

(Professor – student conversation ends)

In batch reactor

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you are not allowing those fellows and then you are waiting for either 10 seconds or 20 seconds or 100 seconds, you are arresting them. They have to be there. Ok. Whereas here by definition, for reaction to occur, certain reaction, that means 90 percent conversion or may be 80 percent conversion to occur you also need certain time here, right?

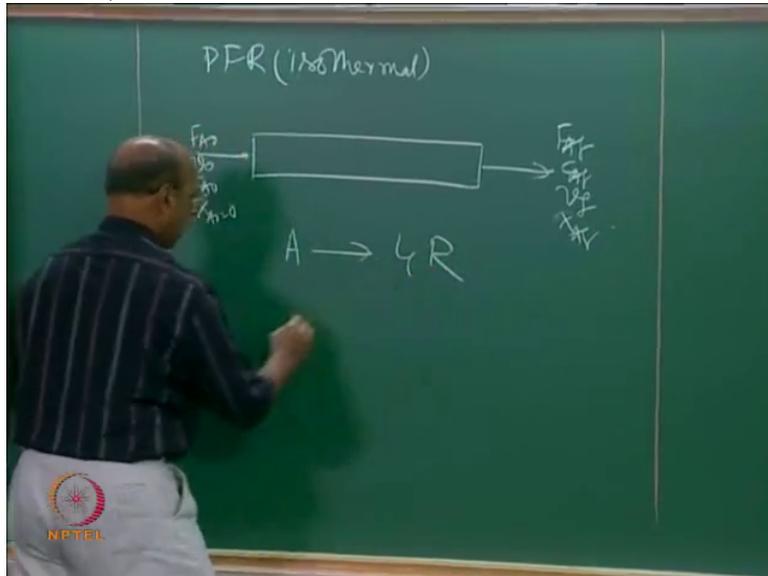
And by the definition of plug flow, all the molecules have to spend; have to spend exactly same time in the plug flow. Whereas in the batch reactor there is no way for the molecules to escape. That is why all of them have to spend exactly again 10 seconds to get this 90 percent conversion. That is the timings.

That is the reason why this can be simply replaced by a batch reactor if we have a constant density system. What do you mean by variable density system, particularly for gas phases, and all liquid phases can be taken as constant density system.

That is why in the examination, I am also giving some clues in the examination. If I say that, liquid phase reaction taking place in a plug flow reactor that means we are talking about constant density system, Ok. Good. So in variable density system particularly for gas phases,

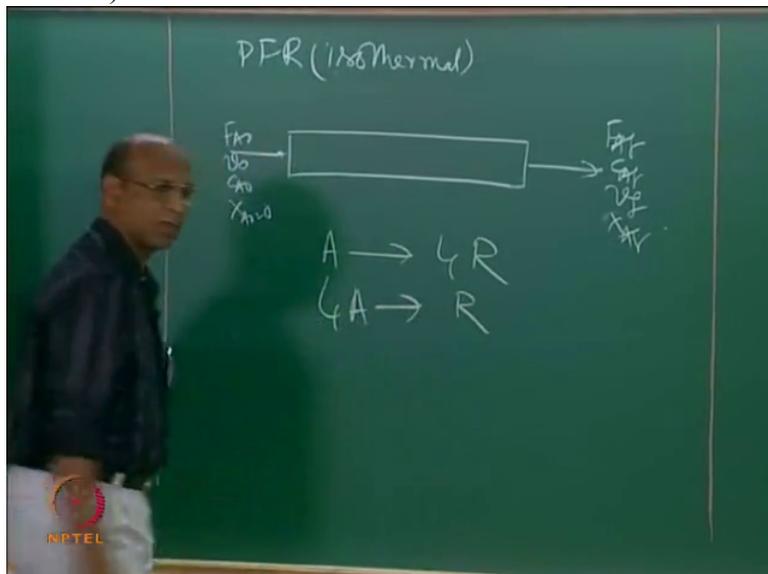
I mean gas phase reactions, when there is difference in moles. That means 1 mole giving 4 moles. Or

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this may be reverse also.

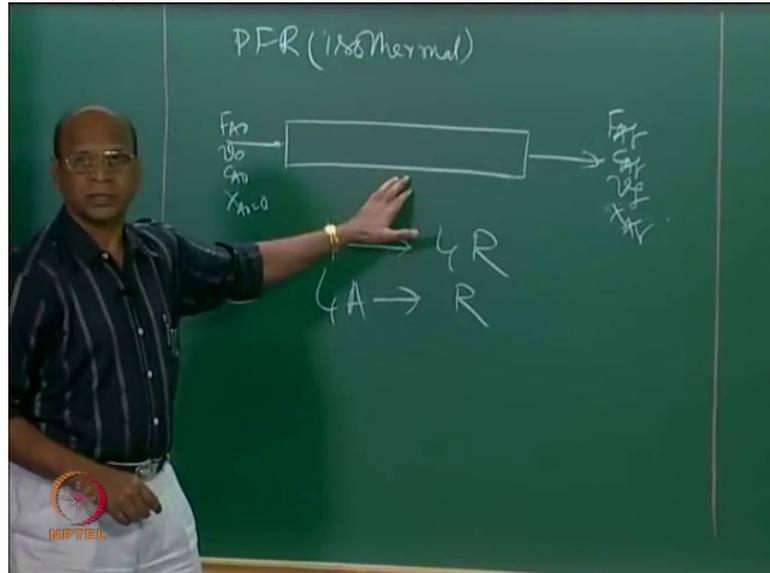
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This is also density, change in density but here you will have less volume at the end because 4 molecules giving you 1 molecule here whereas here 1 molecule giving 4 molecules, Ok 4 moles and then you also know that at constant, you know at N T P, S T P, yeah 22 point 4 liters it will occupy, all those things we know, so then we can easily calculate, under given temperature and pressure conditions what will be the increase in volume, Ok.

What will happen now inside plug flow reactor when I have this kind of situation?

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What will happen?

(Professor – student conversation starts)

Student: 0:05:39.8

Professor: No, please remember that in a flow reactor pressure is always taken as constant.

Student: Volume increases

Professor: Volume increases. Pressure increases if you put them and shut them.

Student: Volume increases, time decreases

Student: Decrease the residence time

Student: Kinetics varies

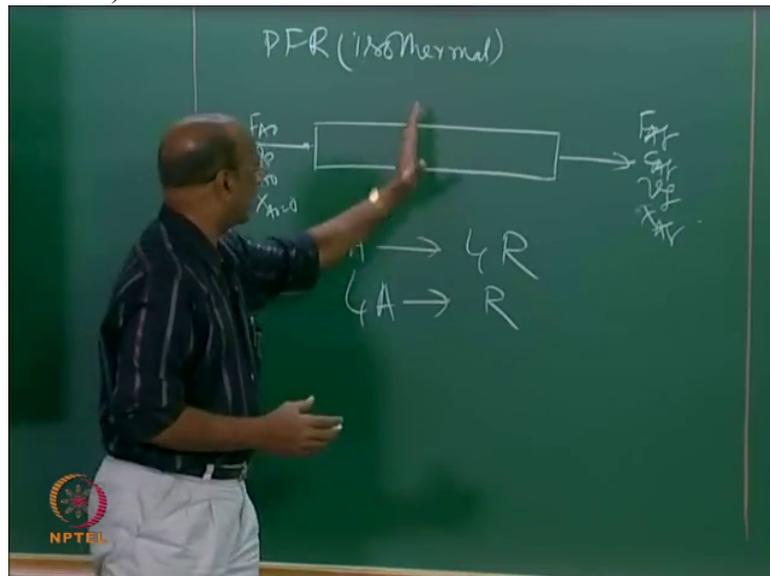
Professor: Yeah the time of flow now changes. Why?

(Professor – student conversation ends)

Because here let us say that also 4 molecules, you know 1 mole giving 4 moles, suddenly all that volume is not increasing. That volume also depends on how much conversion, depends on conversion. If I have 10 percent conversion here, volume expands so much. You can calculate that.

Ok and then if you go slightly inside then may be

(Refer Slide Time: 06:24)



it has come to half, then the conversion is let us say half, for example, 50 percent conversion, you can also find out what is the volume. That volume because pressure is constant throughout, that has to reflect only in acceleration, right.

That has to, because there is a way now for the molecules to escape. Because there is a continuous flow. On the other hand in a batch reactor, same reaction I conduct, right. So 1 mole will give me again 4 moles there. No escape. So everything is shut. And constant volume because I am taking rigid batch reactor, rigid that means walls are very, very strong.

So then what will happen now? Pressure increases. In fact that is the technique used by Levenspiel to measure for gas phase reactions kinetics. You can now find out depending on conversion what is the increase in pressure, not volume, batch reactor, total, total pressure. Now from total pressure, if you know the components you can find out partial pressures.

So using partial pressures and time you can also find out the kinetics, whether the reaction is first order, or zero order or no order at all, and the format of the rate equation you can get from that data. That is why beautifully it is used. And that is also possible; it is a crazy idea, possible to have a variable volume batch reactor. How do I do that?

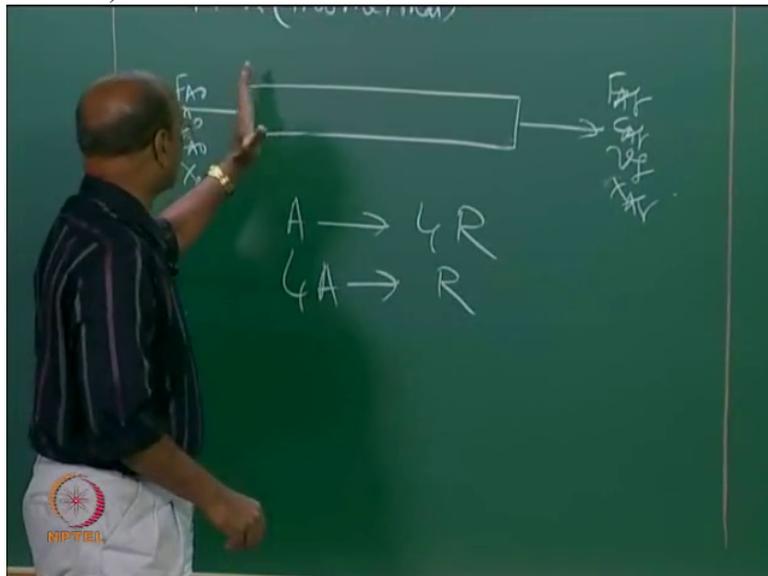
I will take balloon where the elasticity is very, very high, easily it can expand. Elasticity high means easily expands no? Right, expansion. So when I put this one mole and then I have the

conditions for the reaction then the, at the end of the reaction, if I wait for 100 percent almost right, then what will be the volume of the balloon now?

4 times, freely expanding I mean without any resistance. Even that information also can be used for finding out kinetics. And this is what you have already done if you would have used Levenspiel book, I think it is in third chapter, that kinetics chapter where at the end he has given variable volume and also given very nice problems, how do you find out kinetics, how do you find out k values using variable volume batch reactor and also constant batch, constant volume batch reactor.

But here, for our discussion what we have to see here is, when I have

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the gas phase reaction in plug flow, the gas expands and then it moves faster. Ok, so when it is moving faster, then the residence time of those molecules, I mean will be less. So for a given volume, conversion will be less. For a given volume means for a given t value, Ok, yeah, so that also you should have calculated.

That means variable volume what is the conversion, and for a given time for example, or constant volume what is the conversion. Because variable volume particularly when you have 1 mole giving 4 moles what will happen, gas expands, what will happen to concentration?

(Professor – student conversation starts)

Student: Decreases

Professor: Decreases, when concentration decreases, rate of reaction will be...

Student: Decrease

Professor: Less, so when rate of reaction is less, then?

Student: More time

Professor: More time. You see you do not need any expressions at all.

(Professor – student conversation ends)

You do not have to write equation for each and every thing. First like a story we have to discuss. Then if you want to exactly find out, Ok, now what is exact conversion? Or what is exact time for a given conversion?

Then that means number when you come, when you ask then you have to use mathematics. Otherwise to explain subject I do not need mathematics. But please remember, in engineering, mathematics play great role because every engineer has to quantify. Anything you have to quantify, right.

At the end even if you are saying that Ok, my reactor volume is one meter cube, and people will ask you, you know, you cannot simply say that like God, Gods only can say that. Ok, use 1 meter cube, you cannot question them. Because they are Gods.

But if I give that 100 questions will come, why 1 meter cube Sir? Like you already told no, I told 7 meter cube, you say why it is 7 meter cube? You question me. That means to prove that I need mathematics and then I have to say whether you are right or I am right. For that mathematics will come into picture. That is why, mathematics and engineering, inseparable.

Medicine to some extent they can escape, Ok otherwise there are also tremendous amount of mathematics in medicine also when they go to research level. To give Aspirin tablet we do not need any mathematics. Because we also know when to take Aspirin tablet, all of us, Ok even without being doctors, Ok.

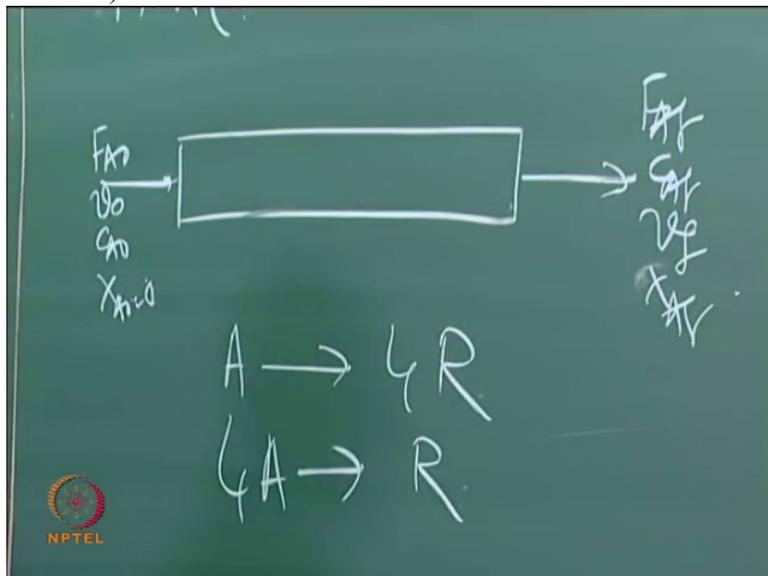
So that is why the mathematics part comes when you want to quantify. Please remember that as engineers. And quantification is a must for any engineer. You have to tell at the end, Ok, so

much is the diameter of the pipe if I use this. I am not talking about reactor, anything. Ok, I think heat exchanger area is this, 10 meter square. How do you get 10 meter square? You have to calculate.

How do you calculate? You have the heat transfer equation, right, design equation. Same thing. Even I think distillation column. Anywhere you go, mathematics automatically comes because you have to finally tell that this is the diameter, this is the height, this is the composition all that. Good, Ok, good.

So now I think you know the difference between the batch reactor and when you will have

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different conversions for a given volume. Or when you have the same conversions, Ok. So that is one information which I want to tell you, Ok. So the other information just,

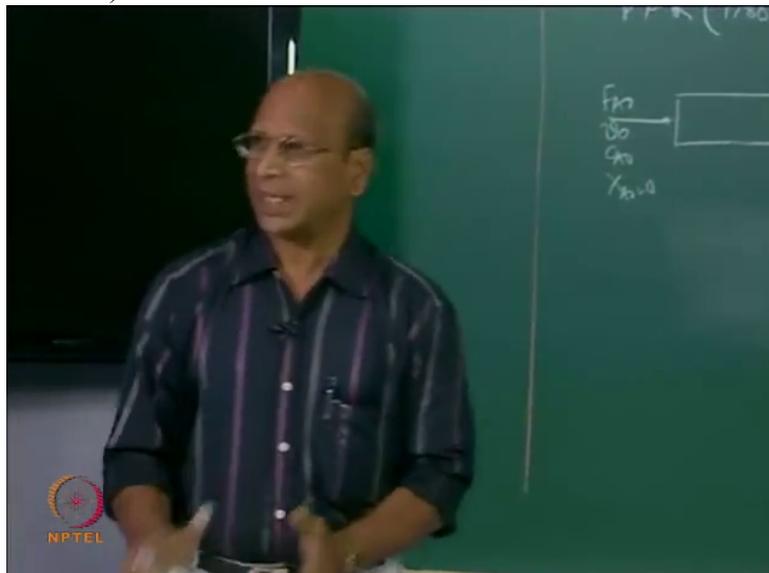
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the design expression for this, right?

The design expression.

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For design expression, now, how do you write the design expression depends on what kind of system you have. Have you heard of what is called distributed parameter system and lumped parameter system? Ok. This comes as distributed or lump? What is distributing there?

(Professor – student conversation starts)

Student: Lumped

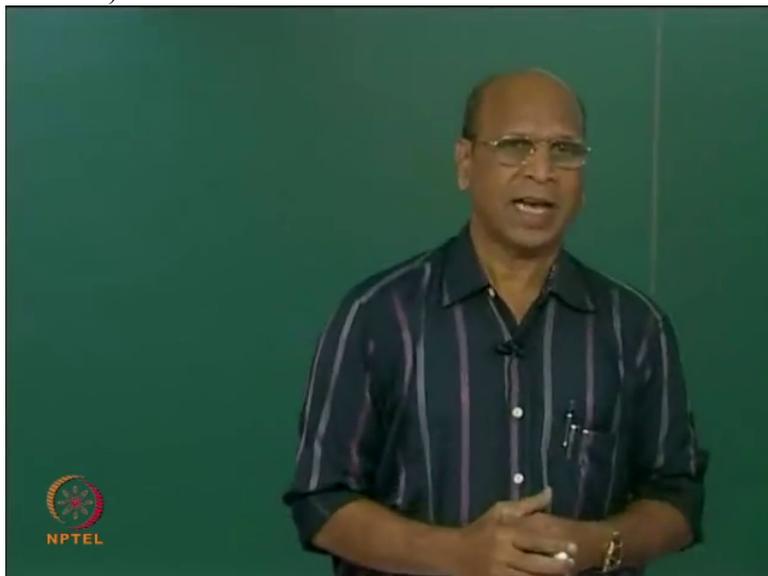
Professor: I want

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you to, you know, I want perfect understanding for you. That is why

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I am asking what is distributing there?

Student: Concentration

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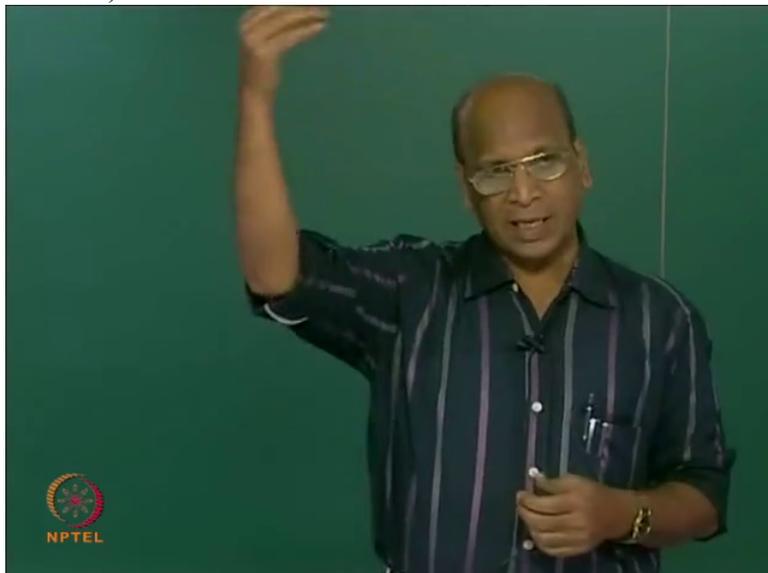


Professor: Concentration and if it is not isothermal, temperature is distributing from this side to that end.

(Professor – student conversation ends)

Whereas

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in a mixed flow reactor when you want to write the balance, so there, yeah only inlet we know what is entering and only outlet we know what is entering, so but in-between if you want to write the balance, you cannot write because there is no change. You cannot see any change.

There is change between inlet and outlet and outlet also will have exactly the same conversions as inside. In fact that is the approach taken by entire B S L. You know who is B S L. You do not know B S L? That you should know. Only you telling very feeble voice, Bird, Stewart, Lightfoot, Ok but I think with louder voice, you know Ok, all of you have used Bird, Stewart, Lightfoot?

Yes, what is the name of the book?

(Professor – student conversation starts)

Student: Transport Phenomena

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Professor: Transport Phenomena, where are these people from?

Student: University of Wisconsin

Professor: Which country?

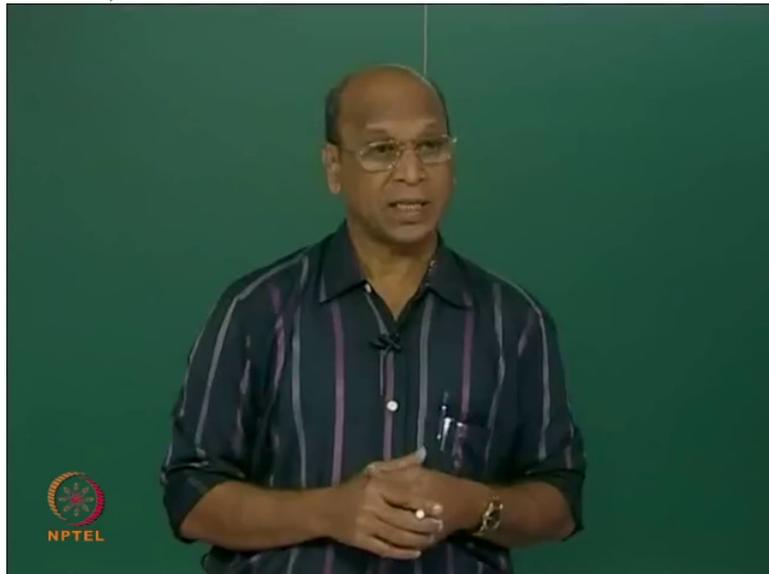
Student: U S

Professor: Ok, good.

(Professor – student conversation ends)

Yeah and when they were

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very young they wrote that book, right? I think all of them were around 30-35. And they changed the thinking of all engineers. It is not only chemical engineers. Even other engineers thinking also they have changed.

Till then everything, I do not say everything but many of the things are only empirical. Doing experimental work, finding out correlation, that is why you have lot of correlations when you are designing heat exchangers, mass exchangers like absorption columns, distillation columns and all that.

These people came and told that even in engineering we can write mathematical equations and then we can solve them and then we can get, you know the concentra/concentration, everywhere you see Bird, Stewart, Lightfoot, there is only one uniform exercises what we do.

At the end what we get all the time is either it is velocity profile, concentration profile, temperature profile, that is all. The moment you know concentration profile, velocity profile and temperature profile, using that, with distance, profile means with distance only, using that you can find out what is called

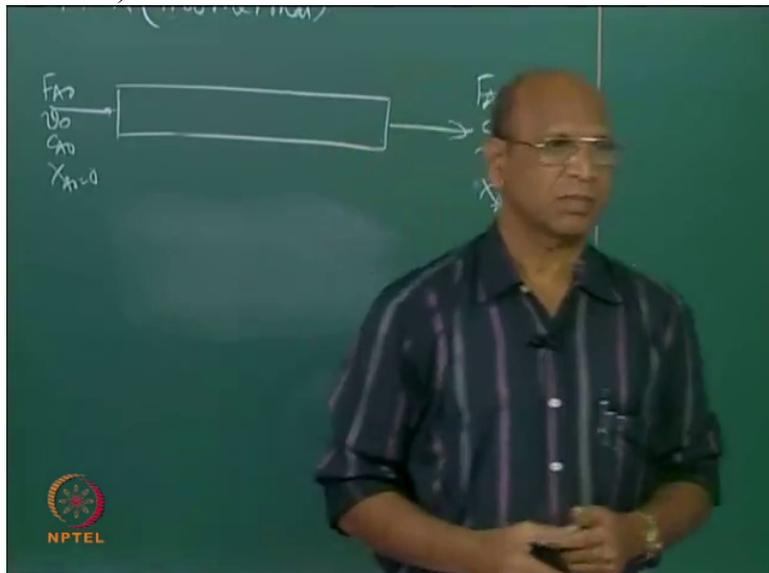
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(Professor – student conversation starts)

Student: Flux

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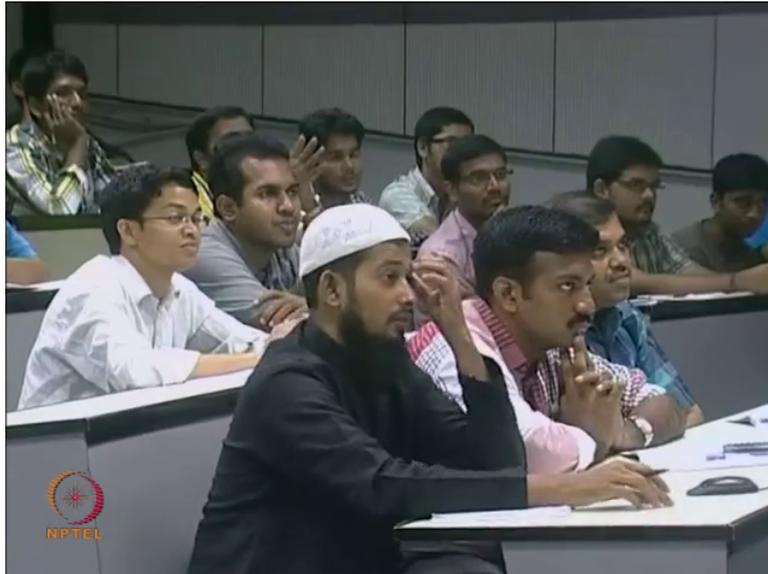
Professor: How do you do that?

Student: Fick's Law

Student: Take the molar weight

Professor: Yeah, you have Fick's Law

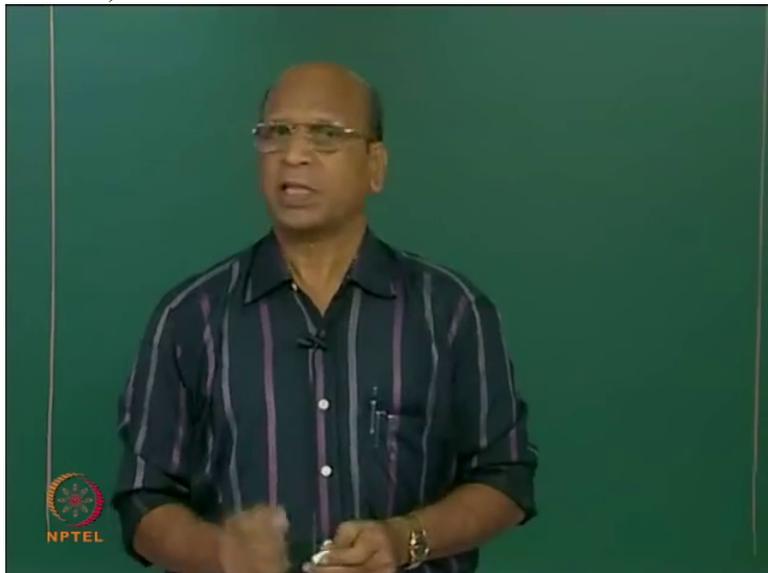
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Student: 0:15:27.7

Professor: That is all. If you now go back and see, the entire book is only that. But the complications

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depend on what kind of balance you write, what kind of systems you take.

(Professor – student conversation ends)

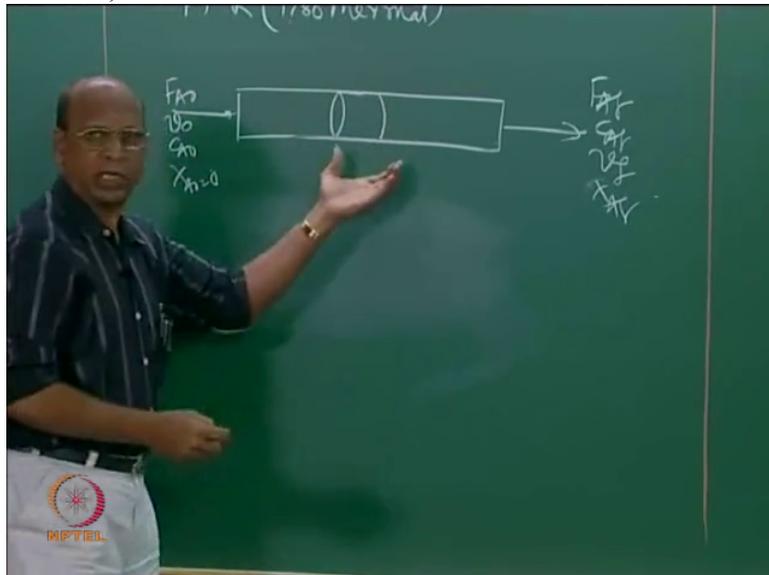
But in the end, all the time again, writing a differential equation and then solving that, and solving as, you know, conversion or some parameter as a function of distance. Of course, unsteady state also you can take, then you will get partial differential equation, partial

differential, that means now that parameter concentration changing with time as well as place. That is all.

The entire transport phenomena is that. But you know the first view is that. But the moment you want quantification you have to take one particular problem, write the material balance, where do you write the material balance and energy balance?

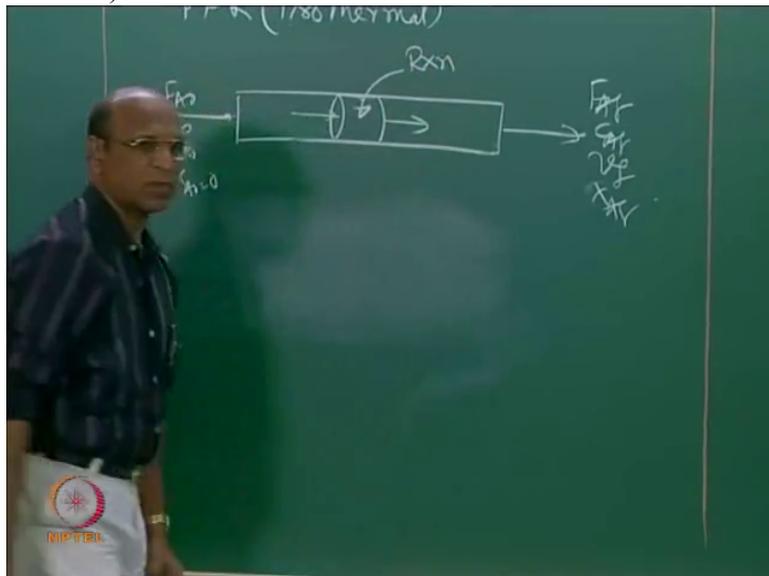
When there is a change you take a small element, that is what what we are going to take now. This is the small, I am showing the big element

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here but that is supposed to be very small element, Ok so then we have to write what is entering, what is leaving, what is reaction

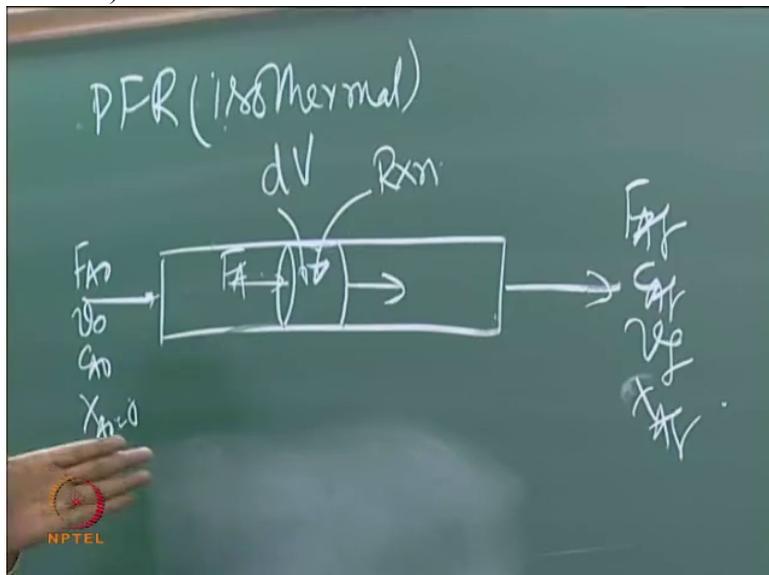
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in that, Ok.

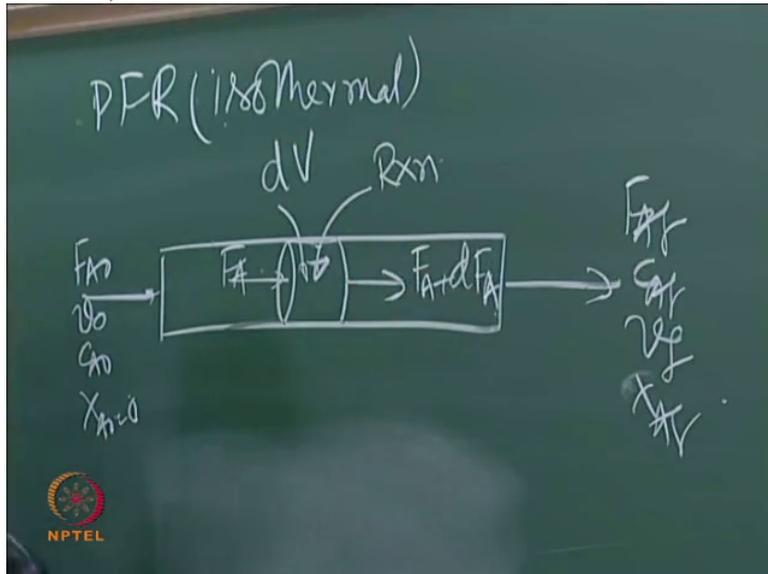
So we call this one as, Ok volume, right this volume is dV , this is $F A$, it is not $F A$ naught, somewhere inside I am taking,

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so this will be $F A$ plus $d F A$, that is very

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simple, Ok dF_A and then now we will, we have to write the overall balance, right and the universal balance what we have, we are only writing for isothermal. So we are only writing for mass.

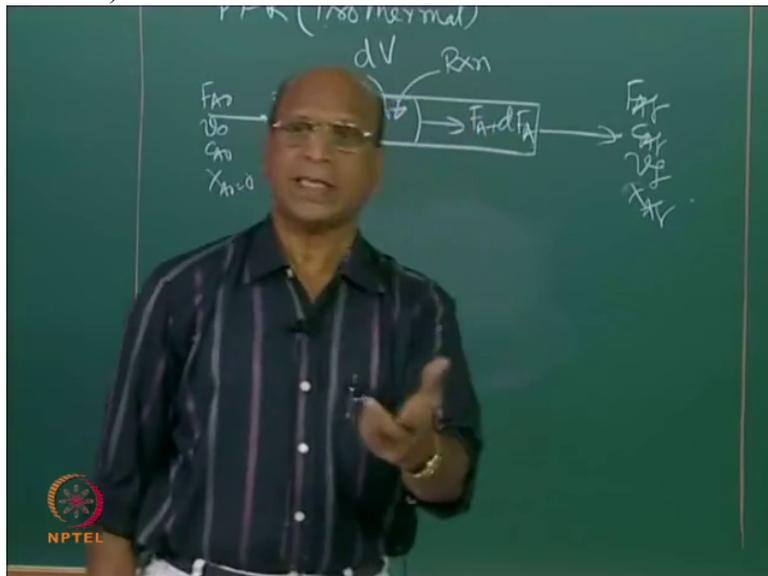
And when you talk mass, we always talk about one particular component, please remember that. I am repeating many times, Ok, whereas for

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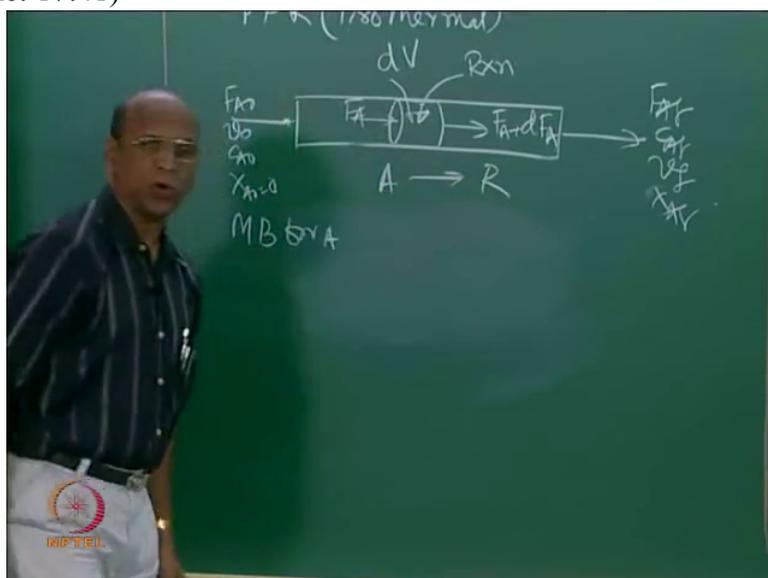
heat transfer

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everything is together, Ok, the entire heat, Ok, good. So now the universal equation for us, M B mass balance for A, if I have a reaction

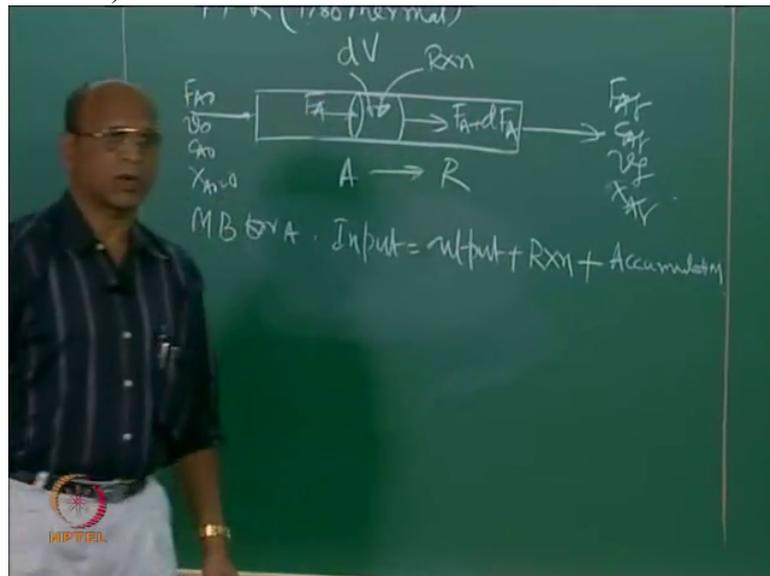
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A going to R. Just I am imagining, Ok, for easy writing.

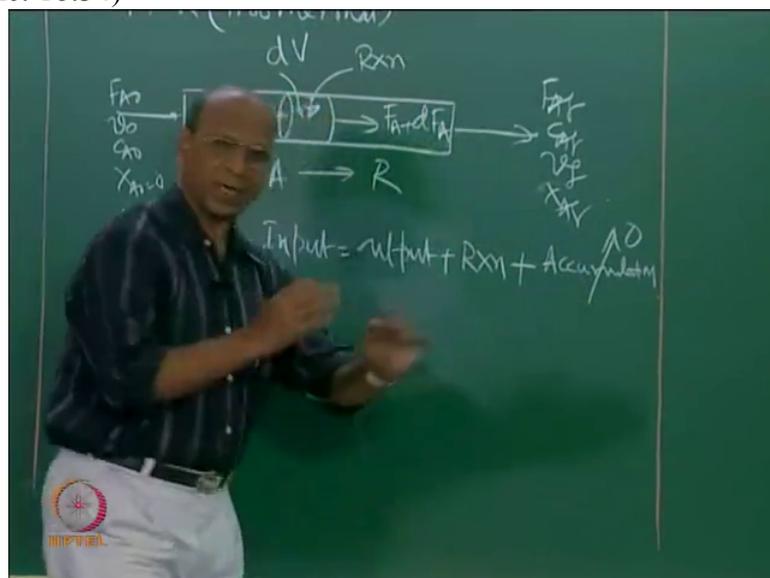
So M B for A is what is entering this element, F_A , Oh sorry I have to write the universal equation first no? Yeah this is input equal to output plus short form reaction plus yeah accumulation. Ok.

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All reaction engineers are steady state people. All process control engineers are unsteady state people because they do not know what is steady state. Ok. So that is why we happily assume that that is not

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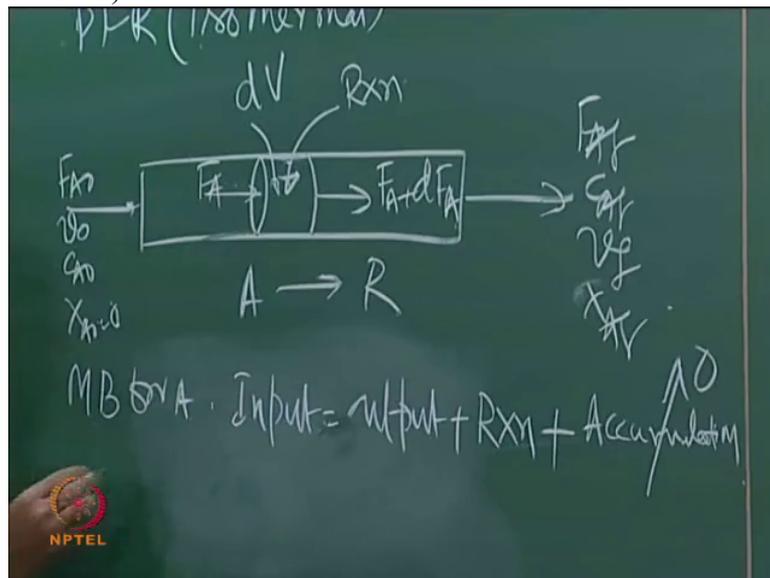
there, right.

So now we have only 3 terms, input, output, reaction. Of course, sometimes this also we have to use, particularly when you are starting the reactor first. You should know under what condi/condition, at what time the steady state comes, for that you have to definitely again solve, but again you will get depending on the equation whether you get unsteady, I mean,

partial differential equation or the other O D E, ordinary differential equation but that will come later when we are talking about Residence Time Distribution

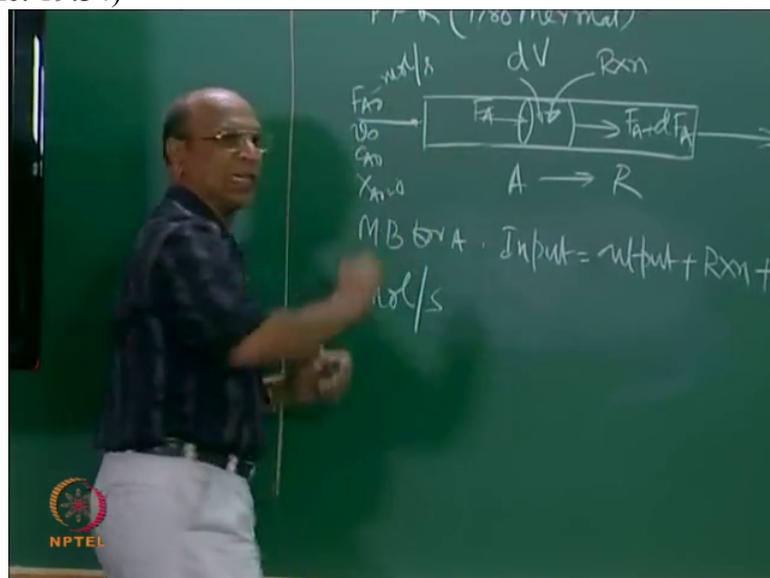
But this is one of the simplest equations what you are going to get. So these moles, M B for A means we are also

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talking about moles per time, may be second. This is better to write in the beginning, right? So now F A according to our notation, Ok, maybe I think some other people are there, so F A is moles per time, moles per second

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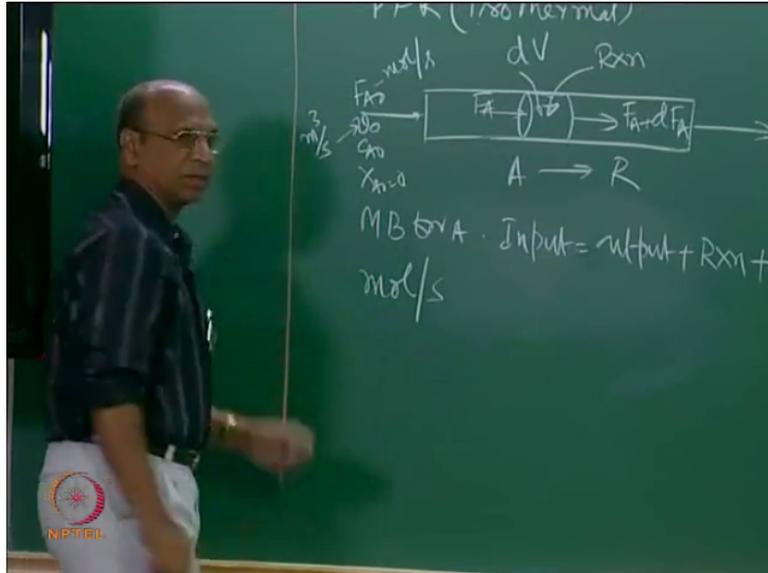
for example. Right and V is

(Professor – student conversation starts)

Student: Volume

Professor: Yeah meter cubed per second.

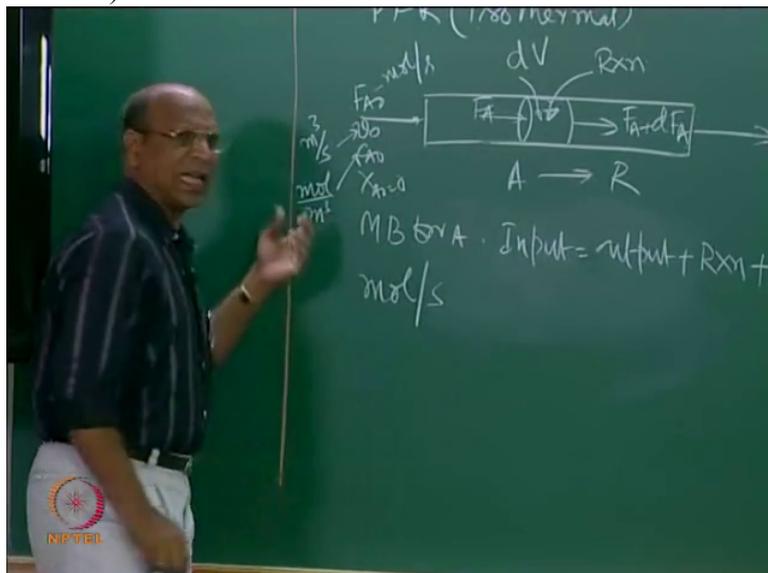
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So this is called volumetric flow rate, this is called molar flow rate. And C_A is yeah, moles per meter cube.

(Professor – student conversation ends)

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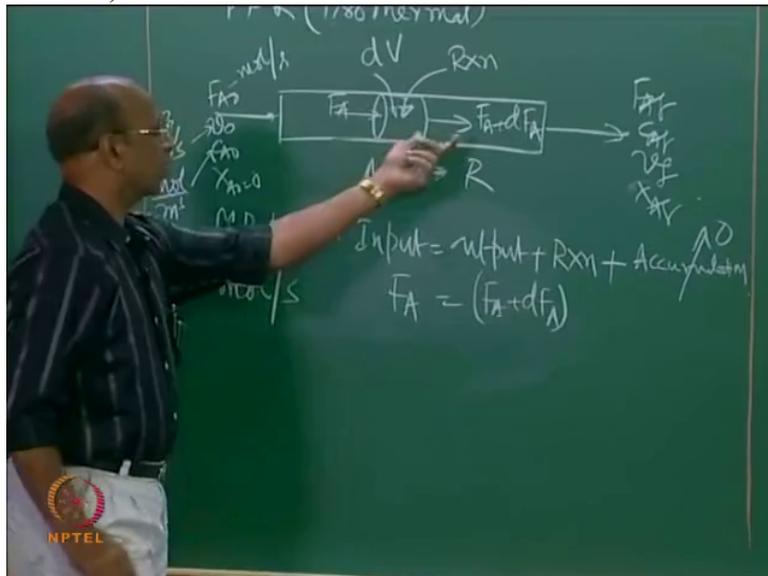


They are not universal. Please do not scold me when I give the problem in kilo moles, Ok. Because I think either kilo moles or moles or lb moles also I can give, pound moles also we

can give. Or meter cubed or feet cubed or centimeter cubed Ok or millimeter cube whatever, right? So this is only per unit volume. And $X A$ naught is conversion where there are no units.

Similarly this side also you have same thing. But we are now balancing moles per second, so I have $F A$ equal to $F A$ plus $d F A$ is the change,

(Refer Slide Time: 20:28)



here, that is the change, either positive or negative, Ok that will come automatically plus we have the reaction. Where is the reaction taking place? That reaction is taking place within this volume. And what are the units of reaction rate?

(Professor – student conversation starts)

Student: 0:20:44.6 per time.

Professor: Because homogenous we are talking right now, Ok so moles per unit volume per

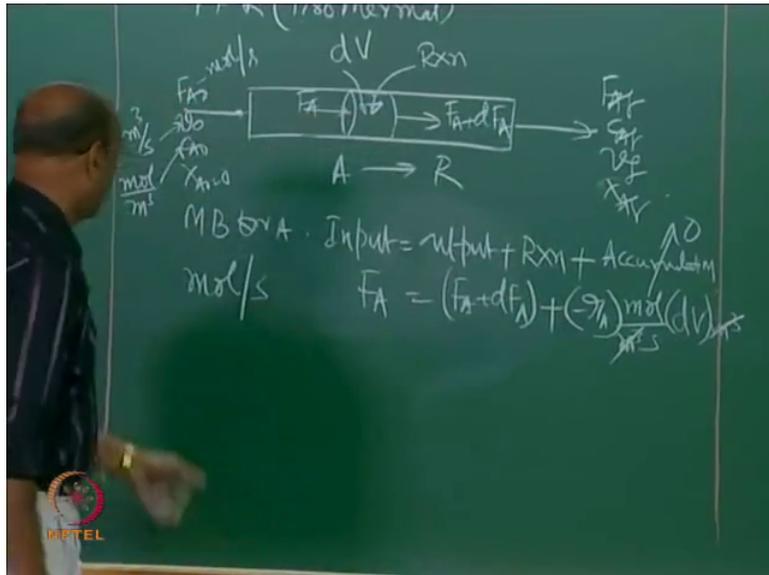
Student: Per time

Professor: Per time. So that is why I will write here our rate is minus $r A$ because always we write A as the key component, this is minus $r A$, and I will also write here moles per meter cube per second into volume is only $d V$. $d V$ is meter cube. Ok, yeah $d V$ is meter cube. So meter cube, meter cube gets cancelled.

(Professor – student conversation ends)

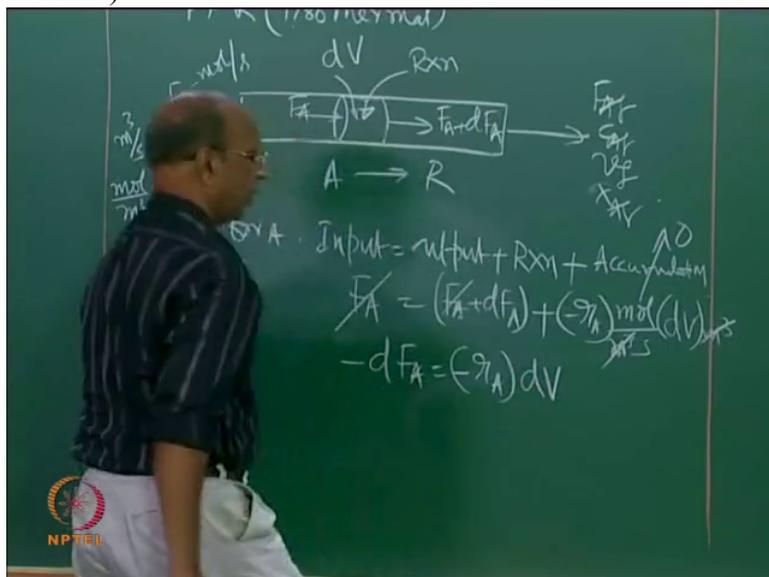
So I will have

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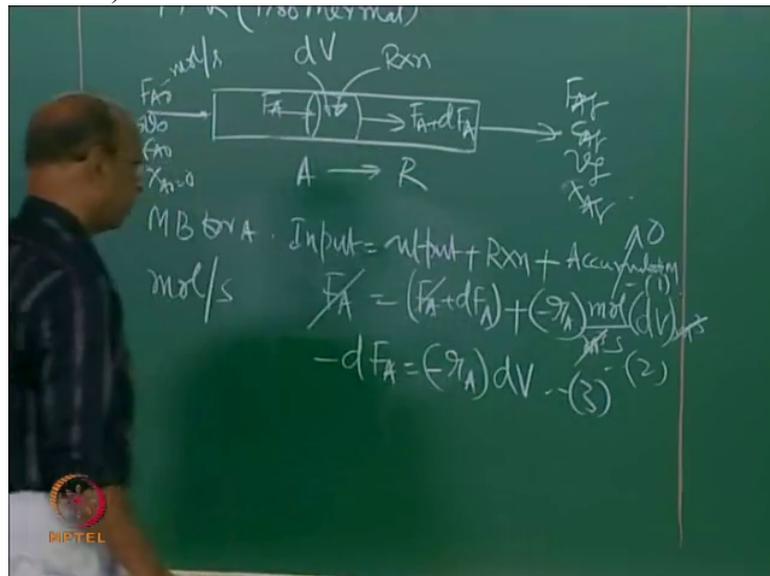
the entire only, moles per second. So my balance is right, right? Ok good. So now this F_A , $F_A + dF_A$ both are same, so I can bring here minus dF_A equal to minus r_A into dV ,

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if I call this one as equation, this is equation 1, this is equation 2, this is equation 3,

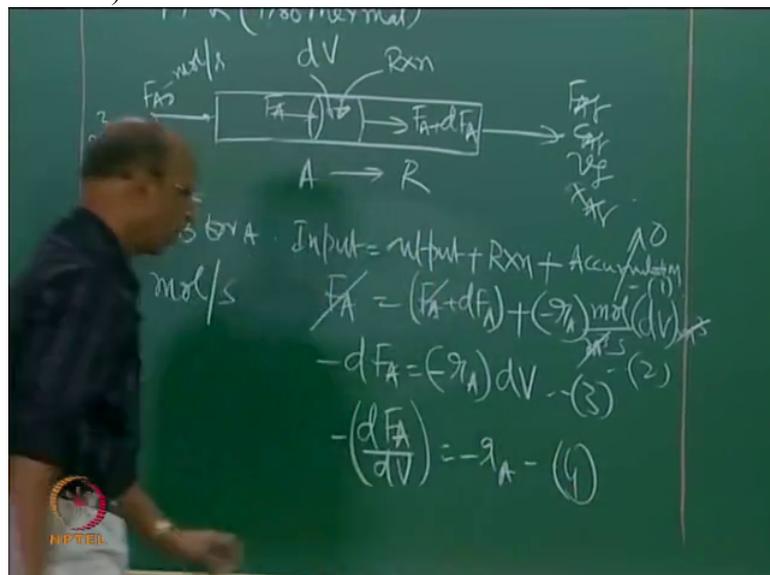
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right?

So in fact I can simply write this equation as dF_A by dV equal to minus r_A .

(Refer Slide Time: 21:59)



By writing this, this equation is not useful to me. Because I would like to put this equation into easily measurable values, F_A is not that easily measurable but I think I want to measure only in terms of conversions, concentrations or conversion, Ok. Good.

So now before going to that, yeah Ok, let me do that and then afterwards we will simplify this. Yeah, so now for flow system, for batch reactor how do you define conversion?

(Professor – student conversation starts)

Student: 0:22:35.4

Professor: For batch how did you define, I think we also told no?

Student: 0:22:38.9

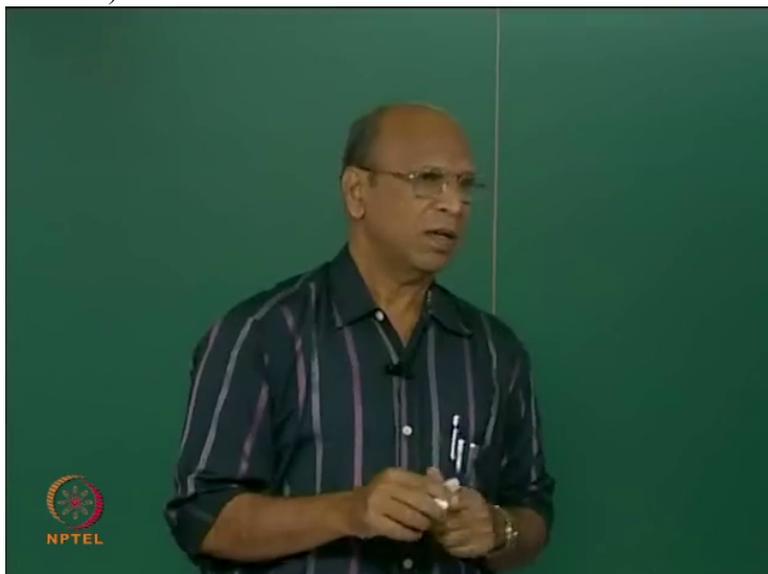
Professor: Yeah, N_A naught minus N_A , N_A naught is initial moles minus N_A is moles at any time,

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N_A naught minus N_A will give you, Arya following?

(Refer Slide Time: 22:50)

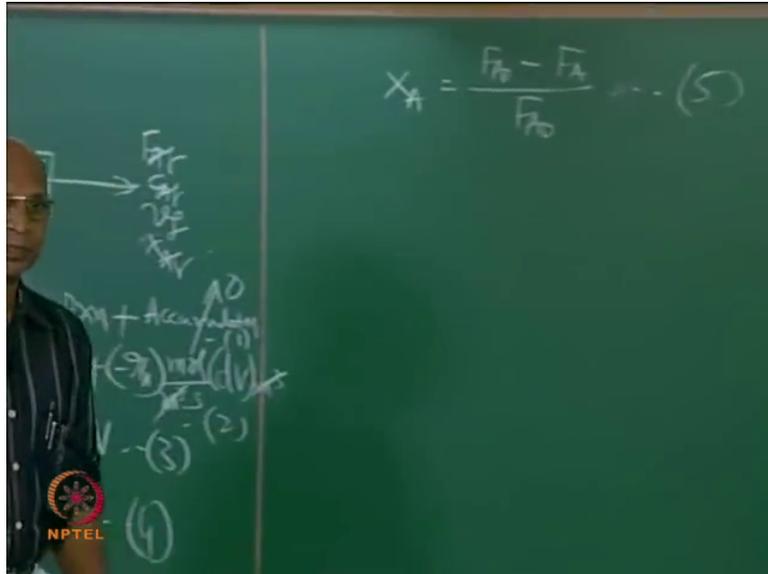


N_A naught minus N_A will giving you moles converted, divided by

Student: Initial moles

Professor: Initial moles, Ok. But for flow system we write the same thing as F_A naught, that is moles per time, there simply moles you are taking. Here per unit time you are taking. So F_A by F_A naught, so this is the definition of X_A , definition of X_A .

(Refer Slide Time: 23:20)



Now from this can you calculate what is $d F_A$? $d F_A$, differentiation, yeah, how much, what you get?

Student: Minus F_A naught into $d X_A$.

Professor: Minus F_A naught

Student: Into $d X_A$

Professor: $d X_A$, you brought this one here, into, minus you put there I think, I will, do not put minus here, minus $d F_A$,

(Professor – student conversation ends)

Ok, yeah, so now this equation 6,

(Refer Slide Time: 23:54)

$$X_A = \frac{F_{A0} - F_A}{F_{A0}} \quad \dots (5)$$

$$F_{A0} dX_A = -dF_A \quad \dots (6)$$

these are very simple but still I am explaining, yeah so now substitute that in equation 3? What do you get? Substituting in equation 3, substituting actually equation 6 in equation 3, minus d F A I will put here, F A naught d X A equal to minus r A d V. So this is the basic equation which we use many times particularly for

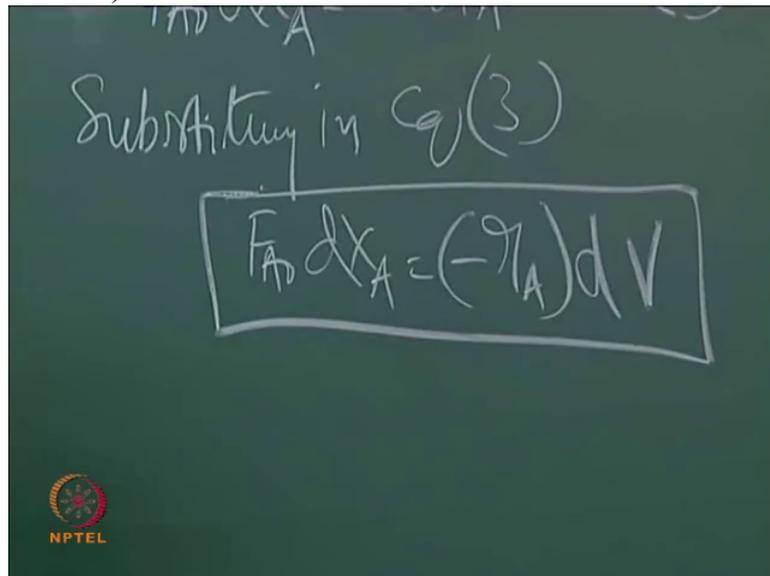
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Prof. K. Krishnaiah
Dept. of Chemical Engineering

non-isothermal systems in differential form.

This is the design equation in differential form.

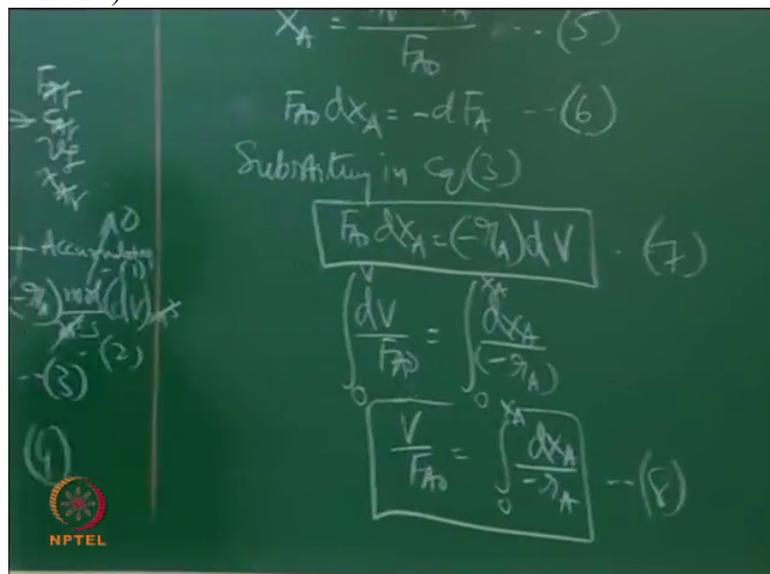
(Refer Slide Time: 24:36)



Ok, yeah. So now we can integrate this. So when we are integrating this what we will change this one is dV by F_{A0} equal to dX_A by minus r_A so integrate. So what are the limits? Zero to V and zero to X_A , right.

So I know zero to V is simply V by F_{A0} , zero to X_A dX_A by minus r_A . So this is the design expression for, this is 8.

(Refer Slide Time: 25:26)



That is design expression for D F R, Ok, the simplest design expression, Ok. Just for comparison we have written for batch

(Refer Slide Time: 25:38)

The image shows a chalkboard with handwritten mathematical equations. The top equation is $\frac{dV}{F_{A0}} = \frac{dX_A}{(-r_A)}$. Below it, the same equation is enclosed in a box: $\frac{V}{F_{A0}} = \int_0^{X_A} \frac{dX_A}{-r_A}$. To the right of the boxed equation is a circled number 8. In the bottom left corner of the chalkboard, there is a small circular logo with the text 'NPTEL' below it.

reactor, what is that?

(Professor – student conversation starts)

Student: C A naught.

Professor: t by

Student: C A naught.

Professor: Yeah, t by C A naught equal to

Student: Integral d X A

Professor: Same, d X A by minus r A, Ok, just for comparison, right, good. That is the one.

So now why this equation become so simple? This is very simple. If I do not assume I have plug flow, because you know... That I have to tell you. Because assumption is one. But you should have questioned me Sir, what will happen if you do not assume plug flow? What would have happened? If there is no plug flow, what is there in the system?

(Refer Slide Time: 26:28)



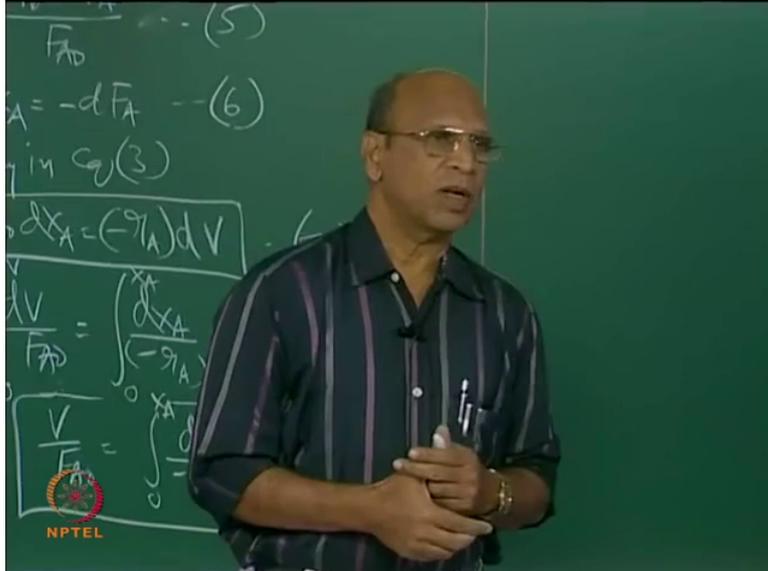
Student: Concentration will change.

Student: There will be no input...

Professor: What Pooja, louder?

Student: Sir no input

(Refer Slide Time: 26:34)



is there so no output will be there.

Professor: We have, we have input and output. It is, it is the flow system but I am not assuming that I have plug flow. If I do not assume I have plug flow, then what is the non-ideality that comes, first non-ideality that comes?

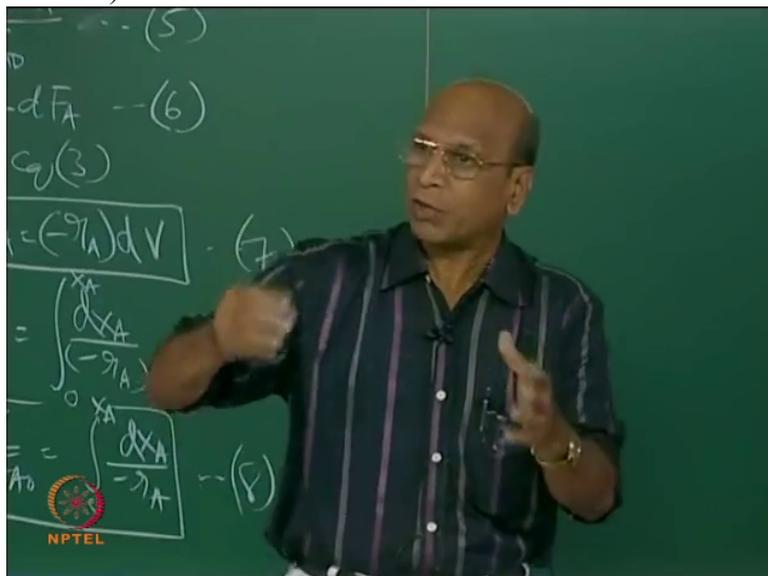
Student: Velocity fluctuations

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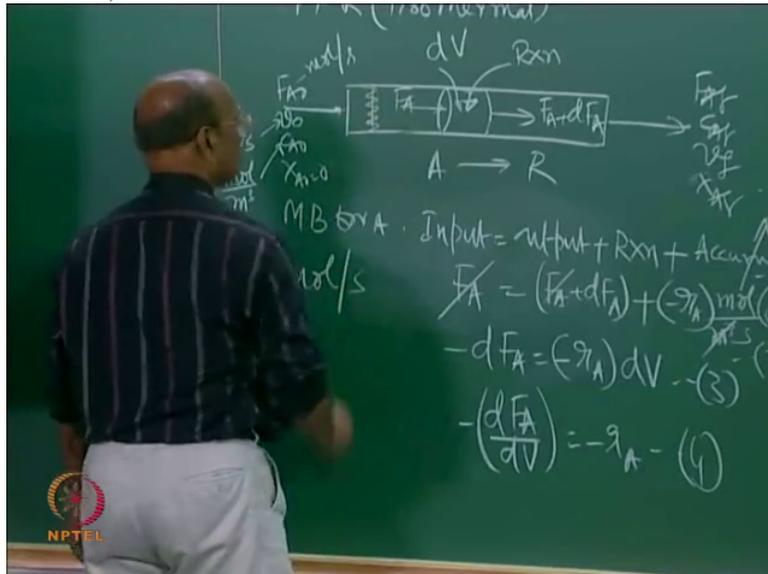
Professor: The velocity fluctuations,

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we are not allowing those fluctuations now here. So the moment we have the velocity fluctuations, how does the, how do they look like? They look like this.

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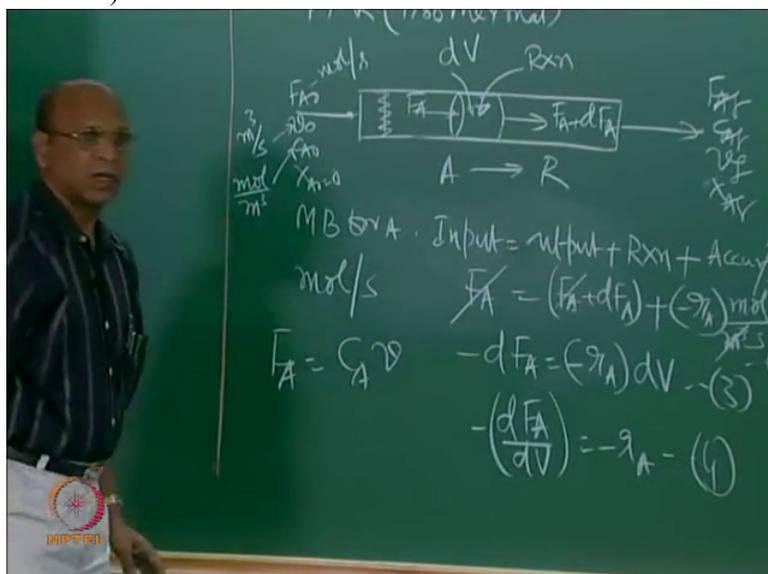


Ok, now, Ok. To bring the point here, I can also write that F_A in terms of C_A , can you write that? Molar flow rate in terms of concentration and, and?

Student: Volumetric flow rate.

Professor: Volumetric flow rate. yeah. So that means I can also write here this F_A as, V into volumetric flow rate into C_{A0} , C_A so where do I write, Ok, here itself I will write.

(Refer Slide Time: 27:40)



You can check the, I think I am worried about Arya and this Chaya, Chaya you are chemistry or chemical engineering? Yeah, you are able to follow? Ok? Yeah, so this concentration you see, because we should help them so, I am just telling even these things, so this C_A what are the units? Arya? C_A , concentration, concentration is always expressed per unit volume, so moles per

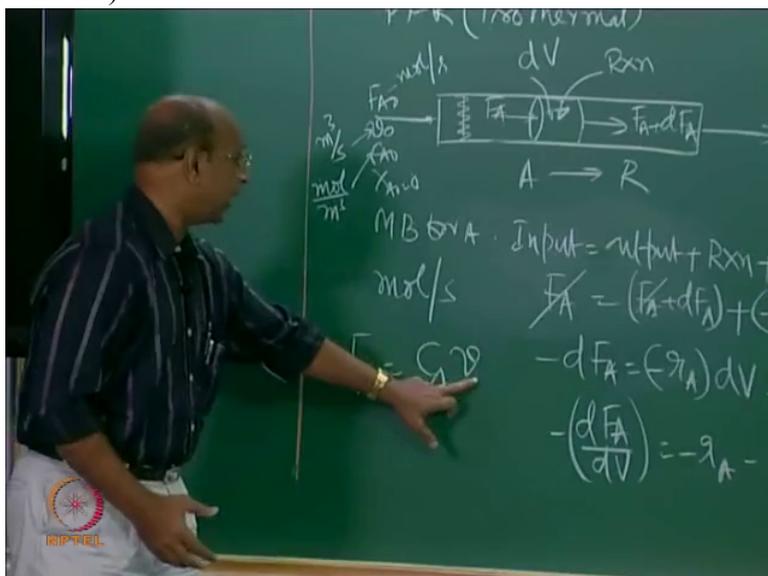
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Student: Meter cube

Professor: Meter cube and this one V?

(Refer Slide Time: 28:15)



Meter cubed per second. You write and tell me what are the units of F_A ?

Student: Moles per second.

Professor: Moles per second.

(Professor – student conversation ends)

So that means even this I can replace by $C A V$. But we wrote directly that because that is the mass balance that gives me. I do not have to use these two very much. But now my biggest problem now is because by assuming plug flow, right, what is the concentration across this?

Uniform C A. If I do not assume that, I do not have uniform C A. Then what is the term I am writing here, this F A?

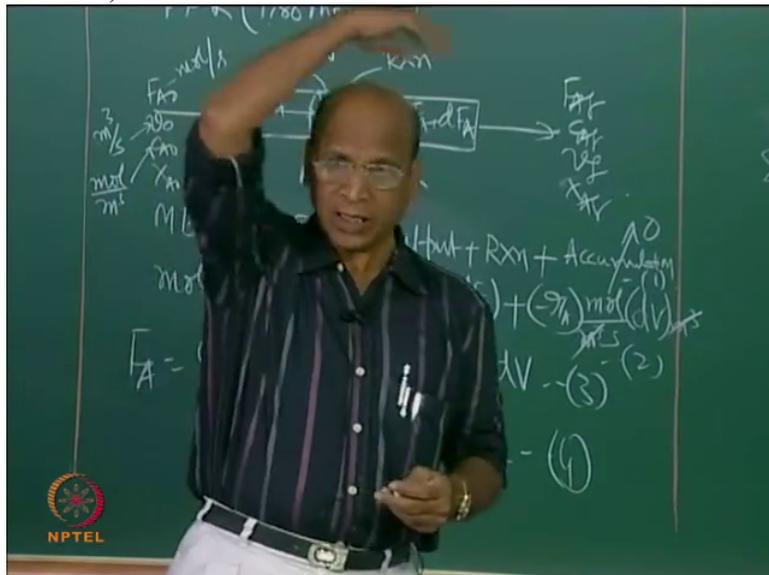
This F A is indirectly C A and V. And when C A is not uniform how can I write that? What concentration I take? Because concentration may be different here, different here, different here, different here. At that cross-section may be different because it is not uniform across the, I mean, cross-section. So then what concentration I can use?

(Professor – student conversation starts)

Student: Average

Professor: What average? How do I know the average? How do you get the profile? You look at all that but that is eating

(Refer Slide Time: 29:26)



like this.

Student: (laugh)

Professor: Yeah, Ok but as an engineer the simplest assumption really we have to appreciate that Professor Denbigh.

(Professor – student conversation ends)

You know Denbigh. Denbigh is the person who has, you know supposed to assume these things. Even mixed flow also, he is supposed who has done that. Actually during Second World War he was working in explosive factory, Ok.

And he was the person who told that, my God! If you use plug flow reactors we will not be here in the company. Because you know temperature control is not that very good in plug flow. Ok. That is why C S T Rs we have to use. And he started using 2 C S T Rs and 3 C S T Rs to produce all explosives. Ok.

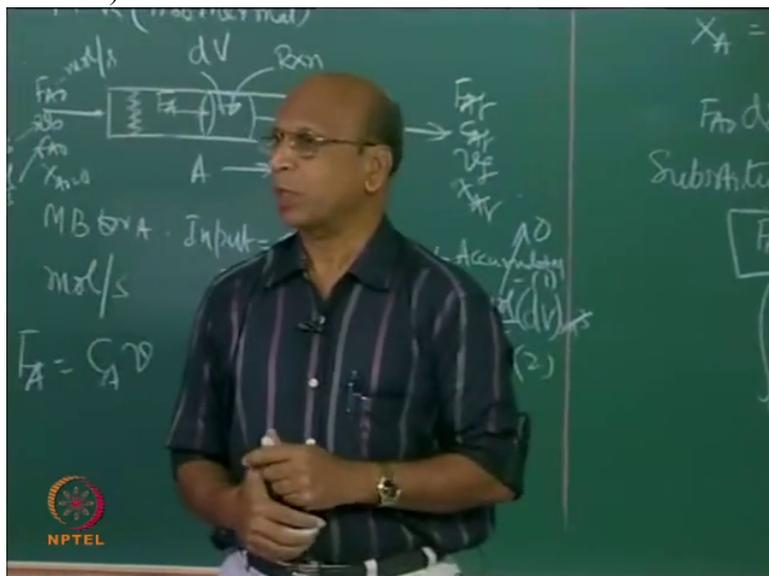
And later he has become great philosopher. Now he is still there I think. But he stopped thinking about research but you know I told you no, that chemical equilibrium,

(Refer Slide Time: 30:20)



Principles of Chemical Equilibrium,

(Refer Slide Time: 30:23)



that book you know, it contains wonderful information about entropy and all that.

The moment you talk about entropy immediately you can see God. Because you do not understand entropy, you do not understand God.

(Professor – student conversation starts)

Student: (laugh)

Professor: So that is (laugh), so that is why both are equivalent. Ok, so that is why now he is trying to find out where is God through entropy. Ok.

(Professor – student conversation ends)

He has become, I think he stopped it seems basic research. But his papers I tell you, I have 1 or 2 papers, I will send it to you but the only thing is I do not want to create e-pollution. Ok, so I do not know how many of you read my Feed the World.

Ok, you see that is what is e-pollution. If everyone reads it, very happy. Otherwise why unnecessarily sending? Otherwise only those people can take from me. Ok. Unnecessarily your computer also is over-burdened. After one day, it may crash, because too many papers and all that.

His papers if you read, throughout the papers I think you know, beautiful logic only. Not mathematics. That is why you have to read that book Chemical Reactor Theory, An Introduction. Even optimization which has maximum number of mathematics in chemical engineering, optimization of chemical reactors, various methods, even there through logic he has found out some conditions for optimality. Later many people used many different mathematical techniques and finally they said that what he has used intuitively was correct. Some condition, at non-isothermal time I will tell you those things.

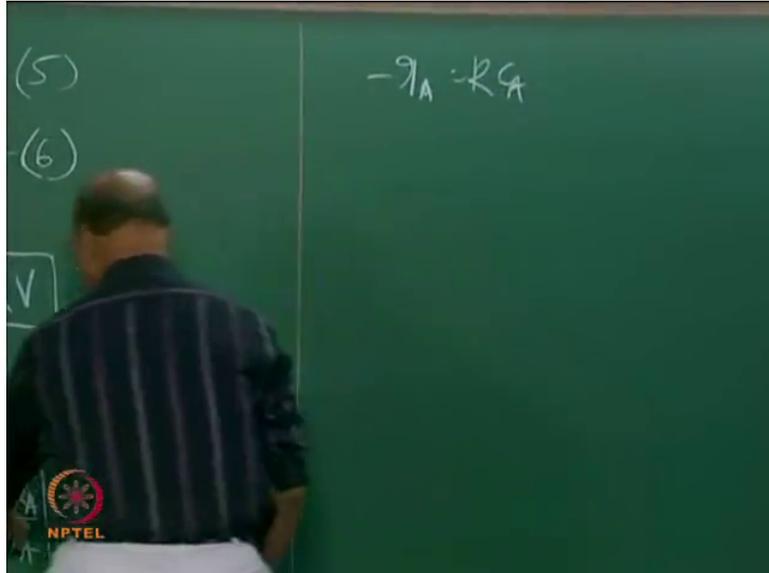
So that is why the beauty of assuming plug flow is that. The moment I do not assume that, Ok, I will also give you an example. Ok. Using this particular, yeah the first thing what I want to tell you is you do not know how to write material balance if do not assume first of all plug flow, right.

But you can also calculate, quantify things, only one parameter if you take, called axial mixing. If you take axial mixing is there and then try to derive the equation and get the

equation for conversion. For first order, what is the equation for conversion here? First order constant density system.

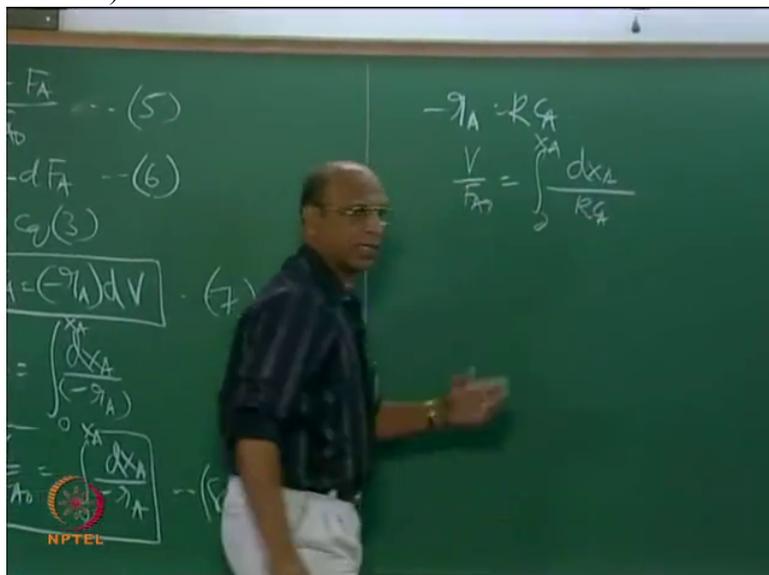
So that means I have minus r_A equal to $k C_A$, so substitute in this equation,

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V by F_A naught equal to zero to X_A d X_A by $k C_A$ right?

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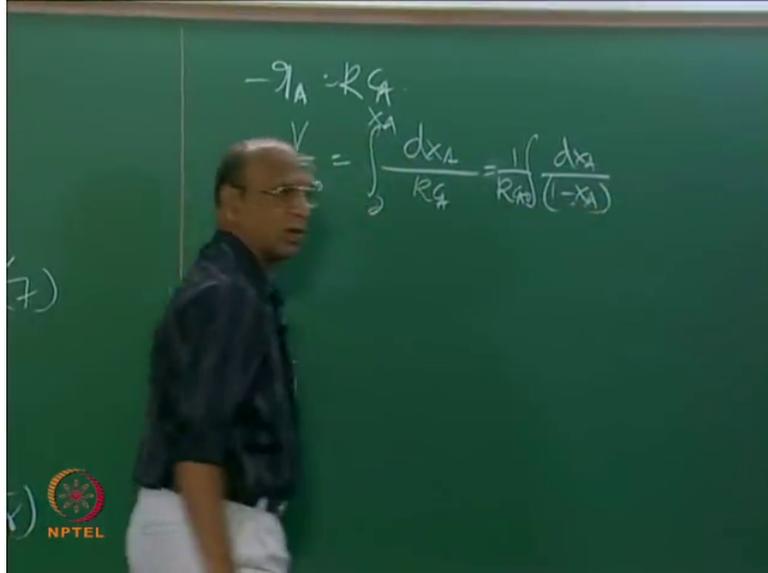
$k C_A$, can I integrate this directly?

(Professor – student conversation starts)

Student: No

Professor: You have to write that in terms of X_A , so that is why I have to write, Ok, constants I will take out, k into C_A naught, $d X_A$,

(Refer Slide Time: 33:09)



it is a constant density system. That is why we said C_A equal to C_A naught into $1 - X_A$, Ok. C_A naught into $1 - X_A$. So now this is equal to what?

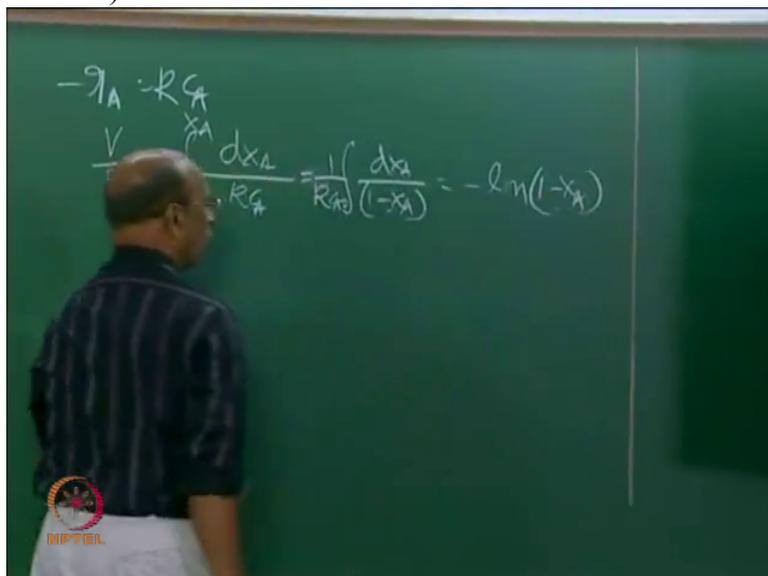
Student: minus log

Professor: Minus log

Student: $1 - X_A$

Professor: $1 - X_A$.

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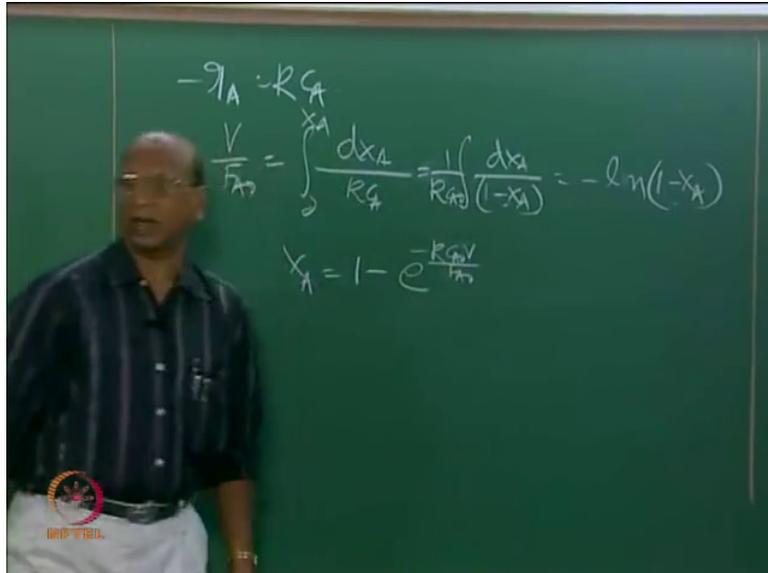


So if I calculate X_A , tell me $1 - e$ power, again minus comes here no? $k C_A$ naught,

Student: V by

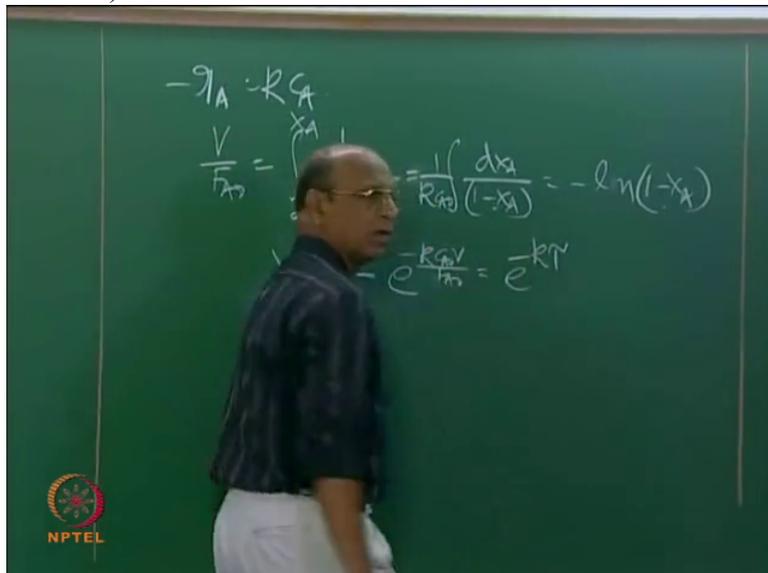
Professor: V by ... F A naught.

(Refer Slide Time: 33:48)



Yeah, actually I do not have to use tau. Really, I think you know the natural design expression is,

(Refer Slide Time: 34:55)



of course, tau if you want to write you can but the natural design quantity is V, the volume. You directly get from these equations the volume itself. Later you want to convert means Ok. So what is tau here then?

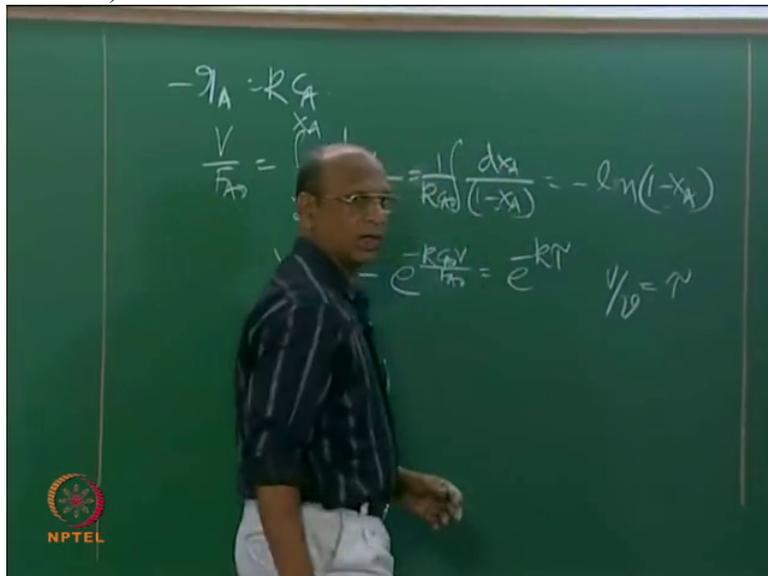
Student: V by 0:34:12.8

Professor: Yeah, F_A naught by C_A naught is V . F_A naught by C_A naught equal to V . So V by v is τ . Then it become $k\tau$, right, yeah.

(Professor – student conversation ends)

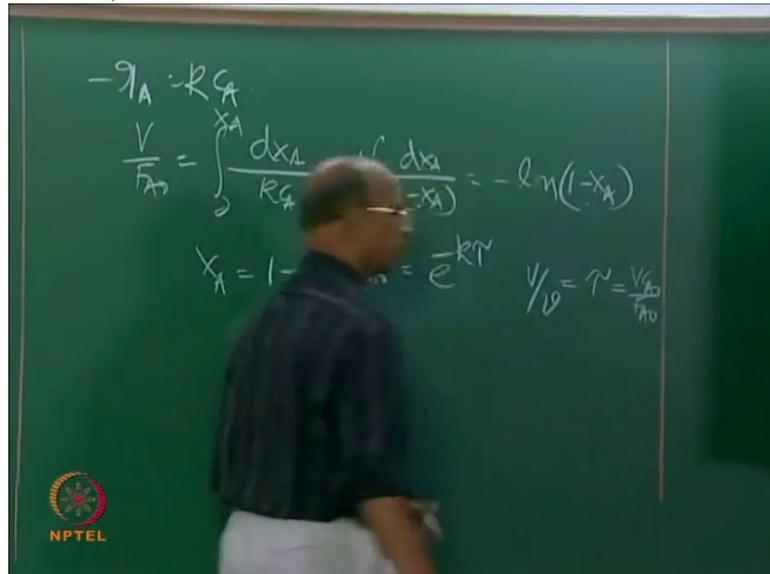
I mean it is easy to remember $k\tau$ instead of remembering another 2 variables. Because you know we should also, we should not strain our minds no? Ok, why unnecessarily remembering unnecessary things? Ok, so that is why if I divide this C_A naught, then F_A naught by C_A naught will give me v , volume by volumetric flow rate will give me τ , so then it becomes k into τ . This will be e power minus $k\tau$ where τ is defined as volume by volumetric flow rate.

(Refer Slide Time: 35:01)



Ok are you able to see here? Yeah, so that is nothing but in terms of, this will be $V C_A$ naught by correct, F_A naught, yeah.

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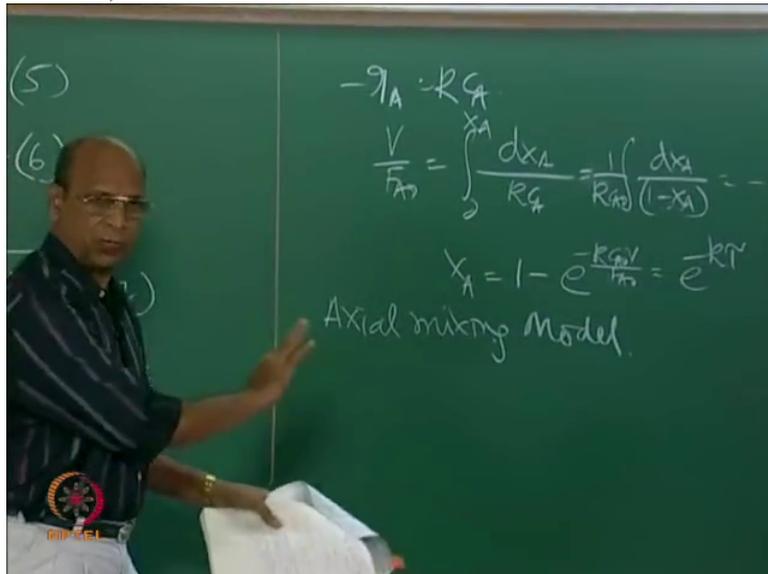


$V C_A$ naught by $F A$ naught, good. Now if you do not assume this, yeah you will get a very simple equation, if you do not assume plug flow and assume the first simplest non-ideality is axial mixing, we are not taking even radial mixing you see, axial mixing is the one where you are getting. But radial mixing also can be non-uniform. Radial mixing, Ok.

So now we are taking axial mixing is one variable first, right. If I take only that, that means I have plug flow, I do not have plug flow but I have axial mixing coming as one of the non-idealities, not ideal. We are calling plug flow as ideal because we are assuming that this is the ideality what should be there. Why? To simplify mathematics. That is very simple.

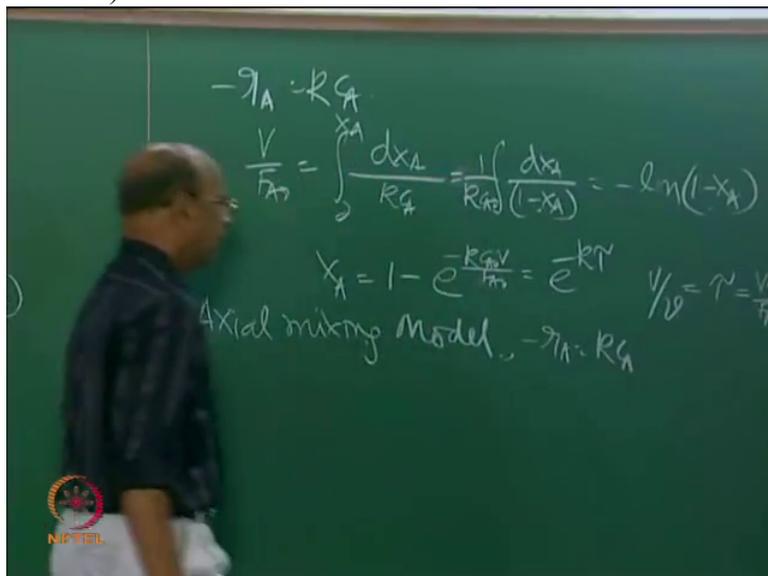
Now you see, with this one, if I have axial mixing model, this is plug flow model, what we have used, this one. Axial mixing model, again first order, same first order,

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constant density system that is why I simply write

(Refer Slide Time: 36:36)



k C A, A going to R, if I use that, then the equation which I get, Ok, the equation which I get is this.

Ok, I think for comparison, anyway I will write this one. 1 minus X A equal to, first of all I have to draw this line. 4 a exponential half u L by d whole thing divided by 1 plus a whole square exponential a by 2 u L by d minus 1 minus a square again exponential, exponential e to the power minus a by 2 u L by d,

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$$-r_A = k C_A$$

$$\frac{V}{F_{A0}} = \int_0^{x_A} \frac{dx_A}{R_A} = \frac{1}{R_{A0}} \int_0^{x_A} \frac{dx_A}{(1-x_A)} = -\ln(1-x_A)$$

$$x_A = 1 - e^{-\frac{kV}{F_{A0}}} = e^{-k\tau} \quad \tau = \frac{V}{F_{A0}} = \frac{V_0}{F_{A0}}$$

Axial mixing Model, $-r_A = R_A$

$$(-x_A) = \frac{4a \exp(\frac{1}{2} \frac{uL}{D})}{(1+a)^2 \exp(\frac{a u L}{2 D}) - (1-a)^2 \exp(-\frac{a u L}{2 D})}$$

very simple expression no? Yeah when compared to this?

If I write this as 1 minus X A, this will be simply e power minus k tau, Ok. So now this e power minus k tau, oh 1 minus e power

(Refer Slide Time: 38:01)

$$-r_A = k C_A$$

$$\frac{V}{F_{A0}} = \int_0^{x_A} \frac{dx_A}{R_A} = \frac{1}{R_{A0}} \int_0^{x_A} \frac{dx_A}{(1-x_A)} = -\ln(1-x_A)$$

$$x_A = 1 - e^{-\frac{kV}{F_{A0}}} = e^{-k\tau} \quad \tau = \frac{V}{F_{A0}} = \frac{V_0}{F_{A0}}$$

Axial mixing Model, $-r_A = R_A$

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minus k tau here, yeah, so now it is not over. Because what is A? You do not know. Ok, so now I have another equation for A.

A equal to square root of 1 plus k tau d by d L, that is the

(Refer Slide Time: 38:22)

$$\frac{V}{F_{A0}} = \int_0^{x_A} \frac{dx_A}{R_A} = \frac{1}{R_{A0}} \int_0^{x_A} \frac{dx_A}{(1-x_A)} = -\ln(1-x_A)$$

$$x_A = 1 - e^{-\frac{R_{A0}V}{F_{A0}}} = 1 - e^{-kT} \quad \frac{V}{\nu} = T = \frac{V_{A0}}{F_{A0}}$$
 Axial mixing Model, $-r_A = R_A$

$$(1-x_A) = \frac{4a \exp\left(\frac{a}{2} \frac{u}{D}\right)}{(1+a)^2 \exp\left(\frac{a}{2} \frac{u}{D}\right) - (1-a)^2 \exp\left(-\frac{a}{2} \frac{u}{D}\right)}$$

$$a = \sqrt{1 + kT \left(\frac{D}{u}\right)}$$

equation and we lost somewhere the numbers, this is 9, 10, 11, 12, 13

(Refer Slide Time: 38:39)

$$-r_A = R_A \cdot (1)$$

$$\frac{V}{F_{A0}} \int_0^{x_A} \frac{dx_A}{R_A} = \frac{1}{R_{A0}} \int_0^{x_A} \frac{dx_A}{(1-x_A)} = -\ln(1-x_A) \cdot (1)$$

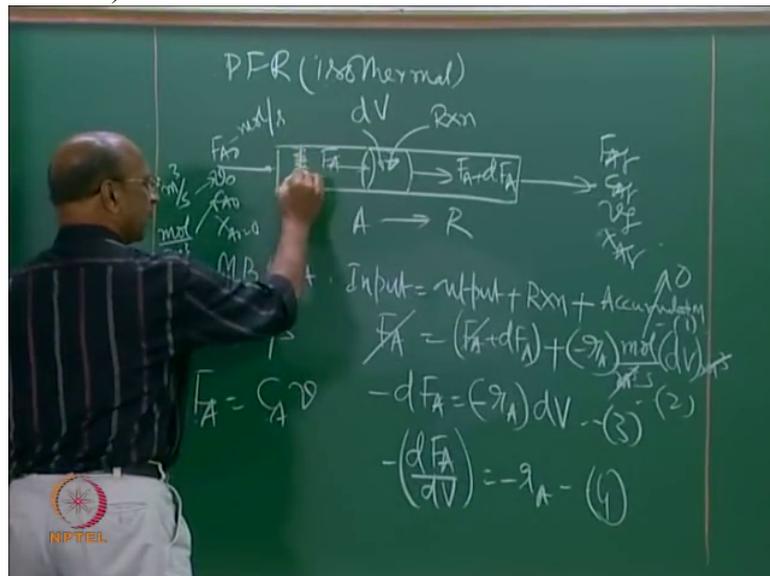
$$x_A = 1 - e^{-\frac{R_{A0}V}{F_{A0}}} = 1 - e^{-kT} \quad (1) \quad \frac{V}{\nu} = T = \frac{V_{A0}}{F_{A0}}$$
 Axial mixing Model, $-r_A = R_A$

$$4a \exp\left(\frac{a}{2} \frac{u}{D}\right) \quad (12)$$

$$\frac{(1+a)^2 \exp\left(\frac{a}{2} \frac{u}{D}\right) - (1-a)^2 \exp\left(-\frac{a}{2} \frac{u}{D}\right)}{\sqrt{1 + kT \left(\frac{D}{u}\right)}} \quad (13)$$

so that is the equation what we have to use if you just consider only one parameter, that is you do not have, you know that means the axial dispersion is always imagined as, we have essentially the plug flow, that is not ideal one but you have some fluctuations over

(Refer Slide Time: 38:58)



that velocity profile, Ok.

That will change. And how do I write this? Because now what is happening is in earlier when I assume, yes this I think I have to discuss, earlier when I assume that I have only plug flow, Ok what mode is the flow inside the reactor? Because flow can happen by diffusion and convection. Diffusion is by concentration difference and convection by...

(Professor – student conversation starts)

Student: 0:39:34.5

Professor: Convection

Student: Velocity difference

Professor: Only velocity? Only velocity. Ok, yeah.

(Professor – student conversation ends)

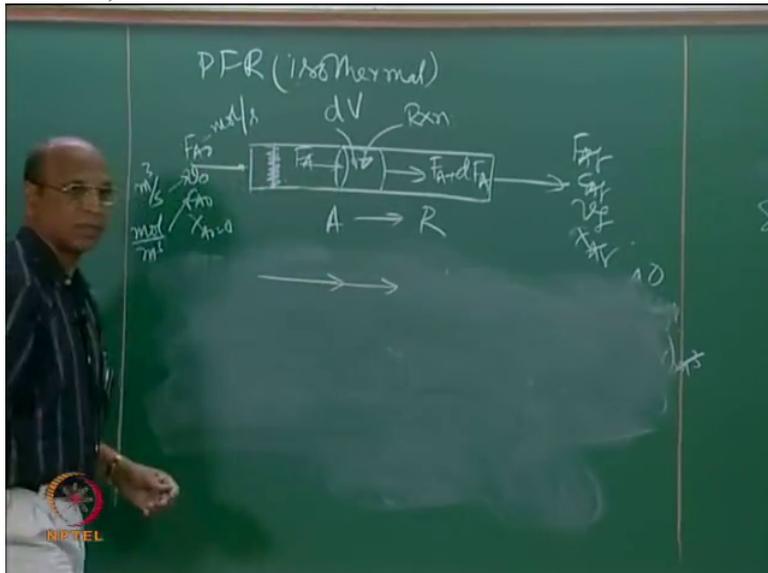
So that means we have now two terms, one is convective velocity, Ok. We will get convective flux. Plus diffusion flux, that is the total flux, right? I will give you a simple example.

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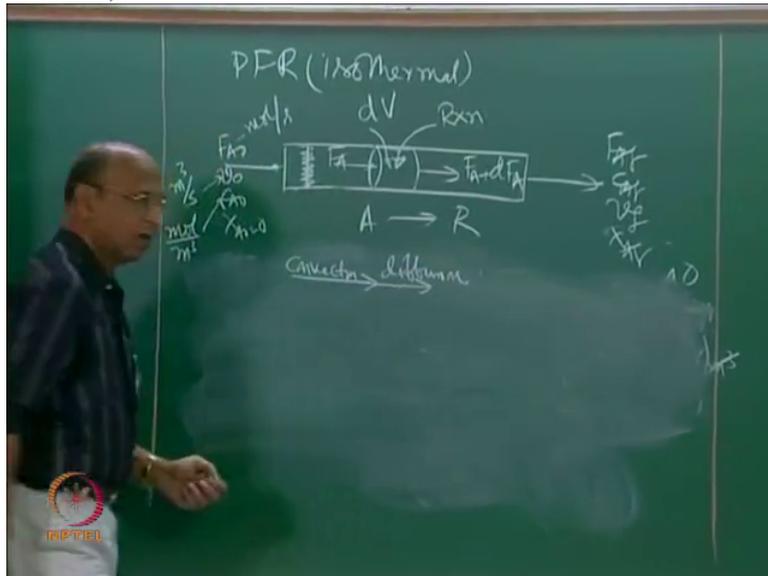
So now I have the diffusion as well as convection both.

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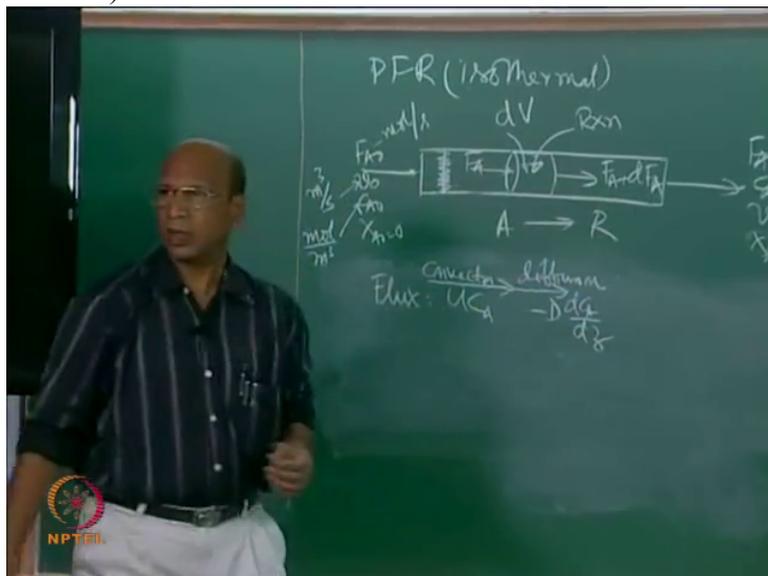
This is convection plus this is diffusion.

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Convection is written as u into $C A$, flux. Yeah, this is minus D , here I can take z ,

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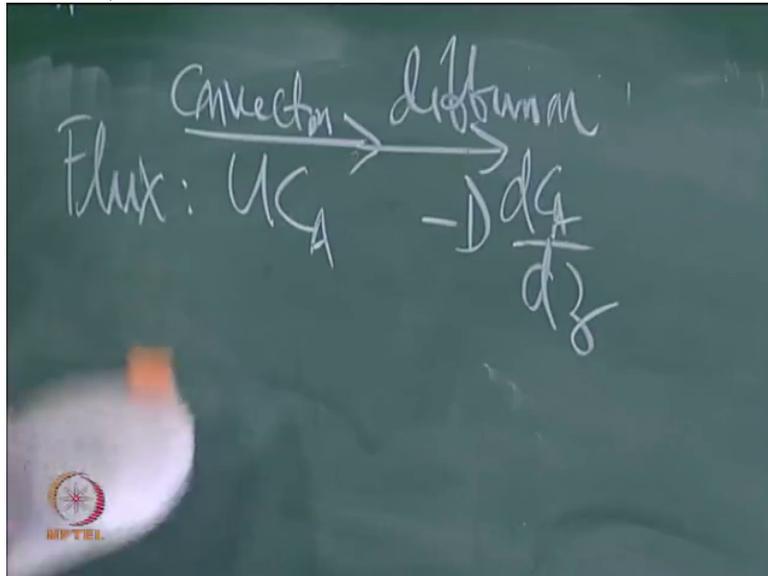


Ok if I take that one as z or x whatever, Ok so this is diffusion flux. So now at this point now I have to write this is the flux no, see here I wrote actually moles per time.

If I take per unit cross-sectional area because here cross-sectional area is not changing. So that is why we are not taking per unit cross-sectional area because it is same diameter, right. But if I take that, that is a flux what is entering here, flux leaving there and then what is the reaction inside. Right?

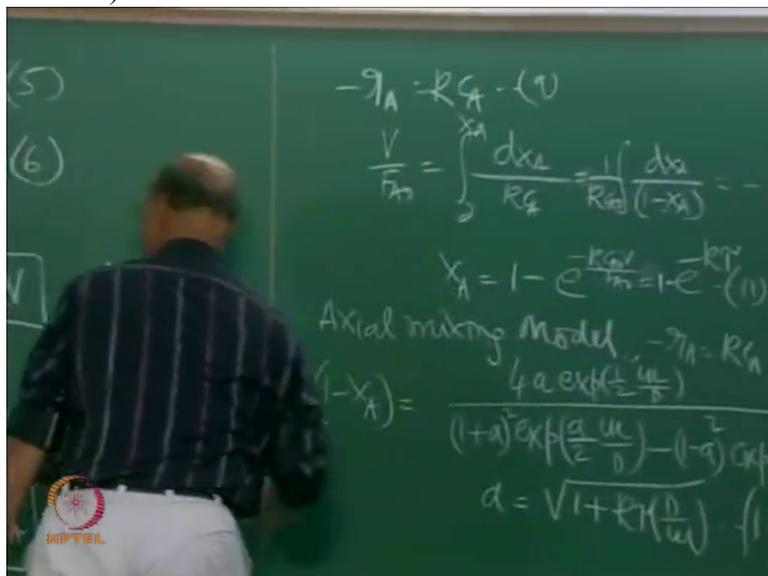
So of course, correspondingly I have to also use this dV , Ok to get again moles per time. So that is why this is nothing but the flux which I have to write here. So these are the two terms now I have to use for solving the equation and the differential equation what you get, yeah for taking,

(Refer Slide Time: 41:29)



by taking you know this reaction and diffusion together where you get this kind of equation

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is

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$$-r_A = R_A \cdot (1)$$

$$\frac{V}{F_{A0}} = \int_0^{x_A} \frac{dx_A}{R_A} = \frac{1}{R_{A0}} \int_0^{x_A} \frac{dx_A}{(1-x_A)} = -\ln(1-x_A) \cdot (10)$$

$$x_A = 1 - e^{-\frac{R_{A0} V}{F_{A0}}} = 1 - e^{-\frac{R_{A0} V}{F_{A0}}} \cdot (1) \frac{1}{D} = \tau = \frac{V_{R0}}{F_{A0}}$$

Axial mixing Model, $-r_A = R_A$

$$(1-x_A) = \frac{4a \exp\left(\frac{a}{2} \frac{u}{D}\right)}{(1+a) \exp\left(\frac{a}{2} \frac{u}{D}\right) - (1-a) \exp\left(-\frac{a}{2} \frac{u}{D}\right)} \cdot (12)$$

$$d = \sqrt{1 + k_1 \tau \frac{D}{u}} \cdot (13)$$

this particular one,

$u \frac{dC_A}{dz}$, this is the convective term, minus $D \frac{d^2 C_A}{dz^2}$ yeah plus $k_1 C_A$ if it is first order reaction equal to zero.

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PFR (isothermal)

F_{A0} F_A dV R_{A0}

$A \rightarrow R$

Convective \rightarrow Diffusion

Flux: $u C_A$ $-D \frac{dC_A}{dz}$

$$u \frac{dC_A}{dz} - D \frac{d^2 C_A}{dz^2} + R_A = 0$$

Ok, what is that I am trying to tell now?

(Professor – student conversation starts)

Student: 0:42:08.4

Professor: Yeah you have to tell now...

Student: Axial dispersion

Professor: See the earlier one which have, axial dispersion model only but why I am telling axial dispersion model at this point of time now; you appreciate the beauty in assumption of plug flow. So what is the differential equation we got for plug flow, pure plug flow?

Student: $0:42:30.4$

Professor: Yeah you see that is dV no, what is that?

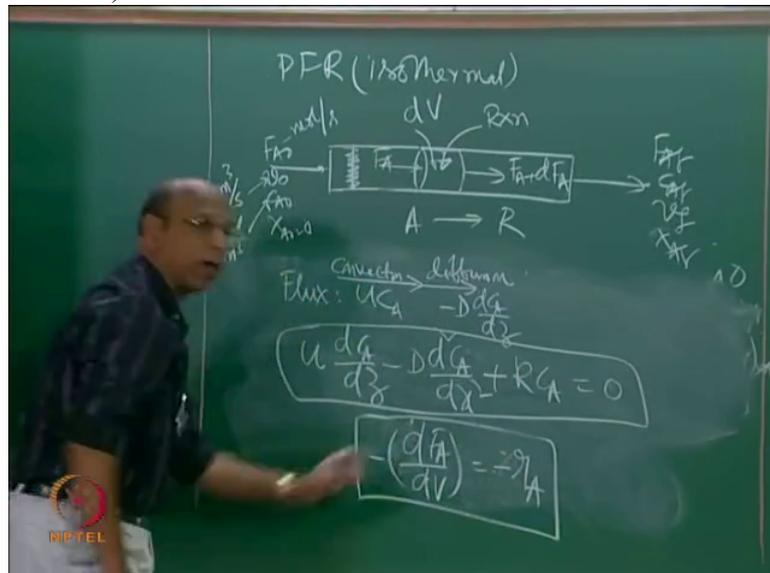
Student: d by $X A$

Professor: No, no. $dF A$ by dV minus equal to minus

Student: Minus $r A$

Professor: $r A$. So this is the differential equation for

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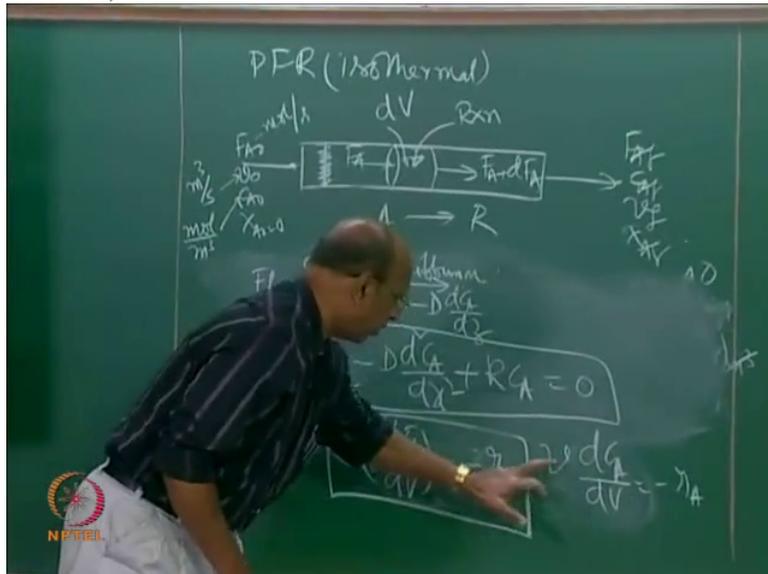
ideal plug flow. I can write this in terms of conversions and all that, concentrations also.

Right. This $F A$ is nothing but...

Student: V into

Professor: V into $C A$. If I take V as constant this also can be written, $V d C A$ by dV equal to minus $r A$,

(Refer Slide Time: 43:13)



right?

Now if I divide by cross-sectional area of this and this? Divide by cross-sectional area of this and this, very simple

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I say this will be velocity and what about this one? Volume, this volume element I am now dividing by cross-sectional area.

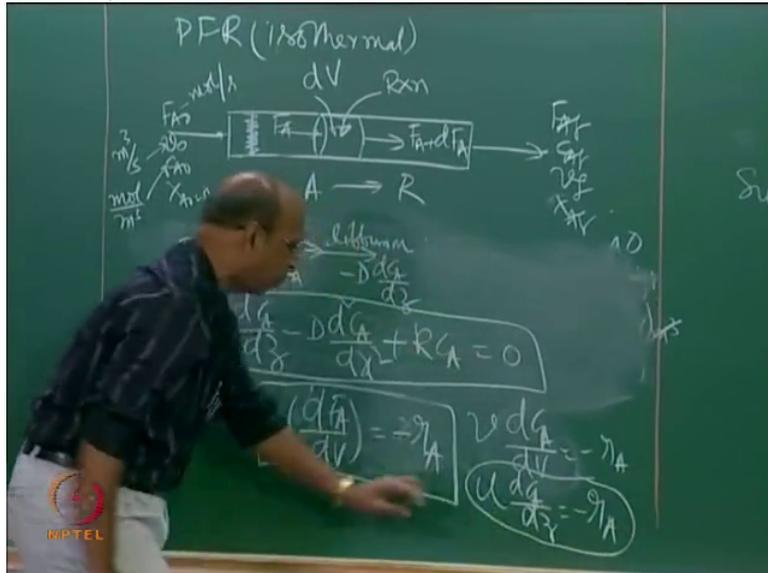
Student: Length

Professor: Yes, now this is $dC A$ by

Student: $d z$

Professor: $d z$ equal to minus $r A$, this is what I want to prove. How simple

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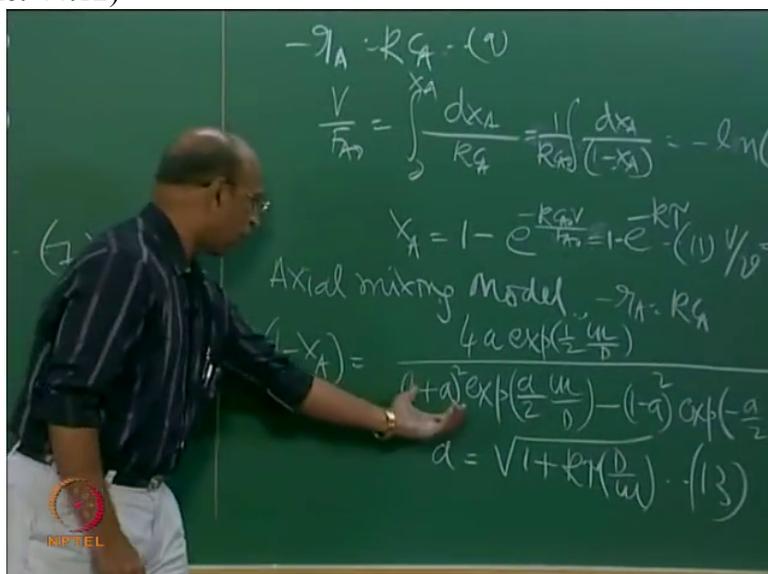
this equation is!

(Professor – student conversation ends)

Whereas this equation, this term. So to avoid this, first we are assuming that we have ideal plug flow. So this, all this last 10 minutes discussion is just to appreciate the assumption of plug flow, right? So for that, to give an example, because example will give you very clear picture what are the complications if you do not assume plug flow? The complication is this. Ok.

This is the

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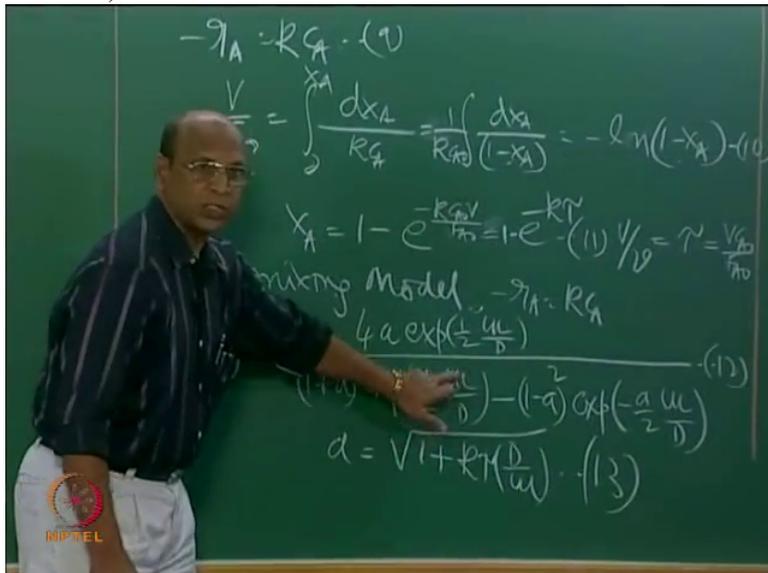
equation what you get for calculating conversion given volume.

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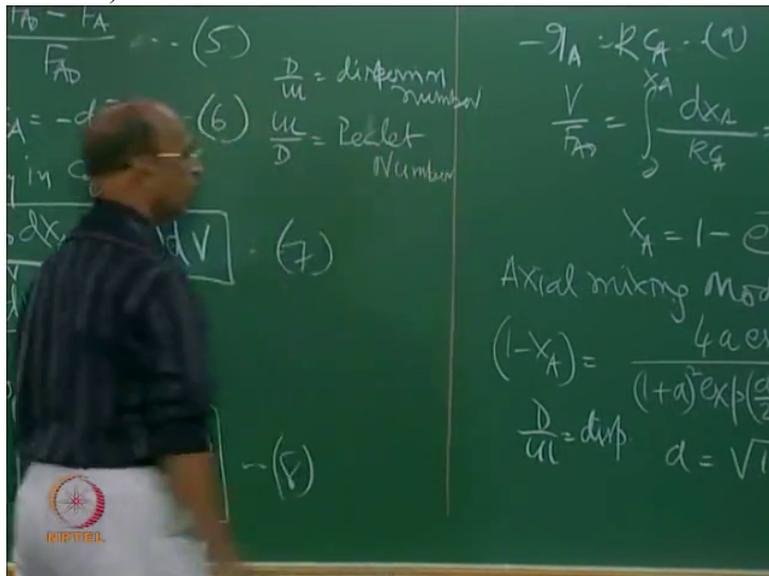
This is called dispersion number. d by uL is

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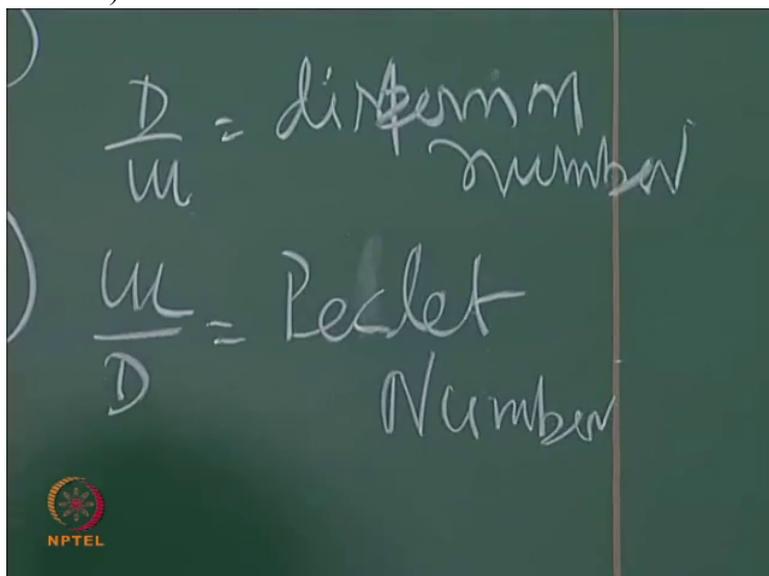
called dispersion number. d by uL equal to dispersion, 0:44:25.2 also, Ok. d by uL is equal to dispersion number. And inverse of this you know, yeah high funda people use this. Peclet Number, they call Peclet.

(Refer Slide Time: 44:48)



u L by d, right? Yeah, that will tell me what will be the dispersion. Like for example when d by L equal to zero what is the system?

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(Professor – student conversation starts)

Student: Plug flow.

M; When d by L equal to infinity?

Student: Mixed flow

Professor: Mixed flow. When Peclet number equal to zero?

Student: Mixed flow

Professor: Mixed flow. Ok, when Peclet number will be zero, because diffusivity is infinity. So that is mixed flow.

And when Peclet number equal to infinity? Plug flow because diffusivity is zero. So you can get all the extremes by these two numbers.

(Professor – student conversation ends)

As I told you high funda people use this, Peclet number, low funda people like me use dispersion number because I do not want to again use another subroutine inside my mind. Dispersion number is straight forward, d by $u L$. d is zero, plug flow, d equal to infinity, mixed flow, right? So that is what I am trying to explain to you.

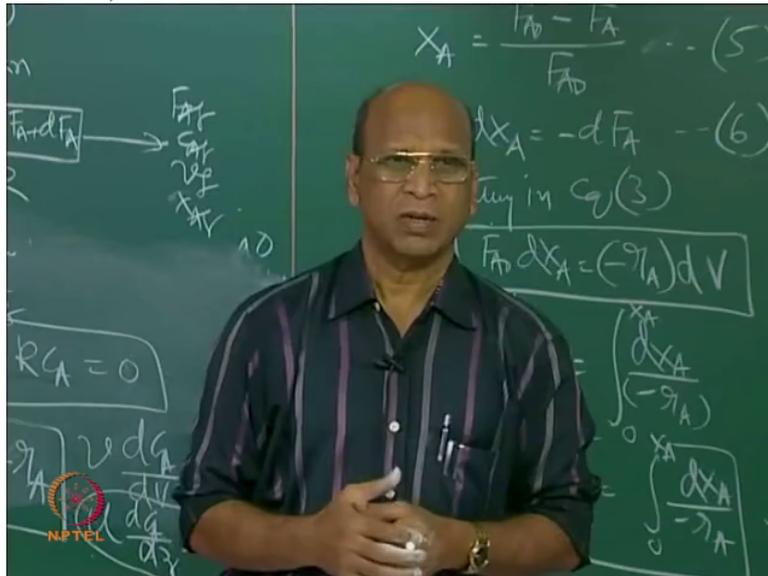
The beauty in assuming plug flow is simplification of, the mathematical simplification of the problem but you have to now my question how far that is correct. Is it really correct? That is correct provided you take small tubes, Ok, diameter may be you know, 1 inch, Ok, around 1 point 5, 2 inches and maintain very high velocities.

The dispersion, there will be dispersion, you can never neglect dispersion. Dispersion will be there. So dispersion is, we have very high, my mind has gone to time so that is why (laugh), Ok so very well valid in packed bed. You know in packed bed, what is the Reynolds number for turbulence?

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No idea?

(Professor – student conversation starts)

Student: 4000

Professor: Ok, tell me when is laminar?

Student: 0:46:44.1

Professor: Then in Stokes law? Only single particle. In packed bed how many particles you will have?

Student: less than 2000

Professor: Yes?

Student: Less than 2000

Professor: Yeah, then why 2000?

Student: 0:46:57.1

Professor: It is 10, 10 and less in a packed bed you will have laminar. And 500 above you have turbulence. In between you have transition. Ok. But here Reynolds number is defined, how?

Student: Diameter of the particle

Professor: How normally Reynolds number is defined?

Student: $d V \rho$ by μ

Professor: $d V \rho$ by μ . Here that d , diameter of

Student: particle.

Professor: There d is

Student: Diameter of the pipe

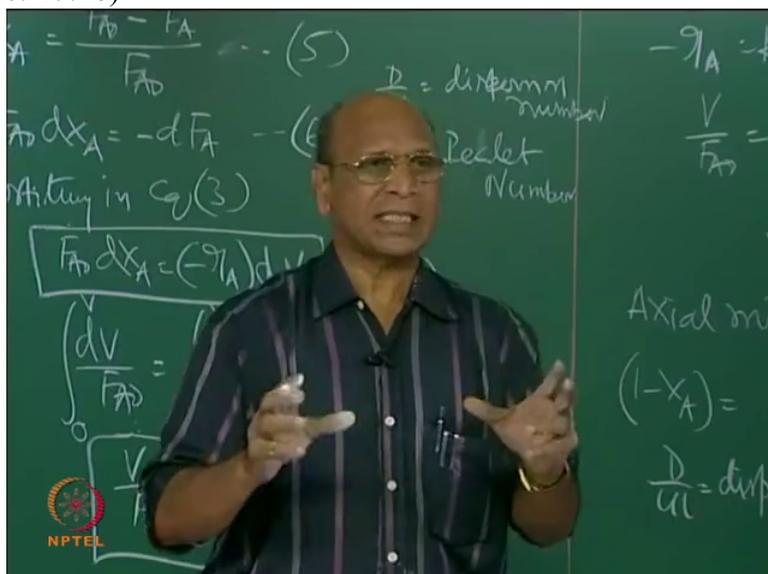
Professor: So that is how it is defined, Ok. So another example, I think today class itself I have to give that is I told you no, diffusion convection. I will give you an example. I think so that you will not forget. Ok, 2 examples I will give.

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Imagine that

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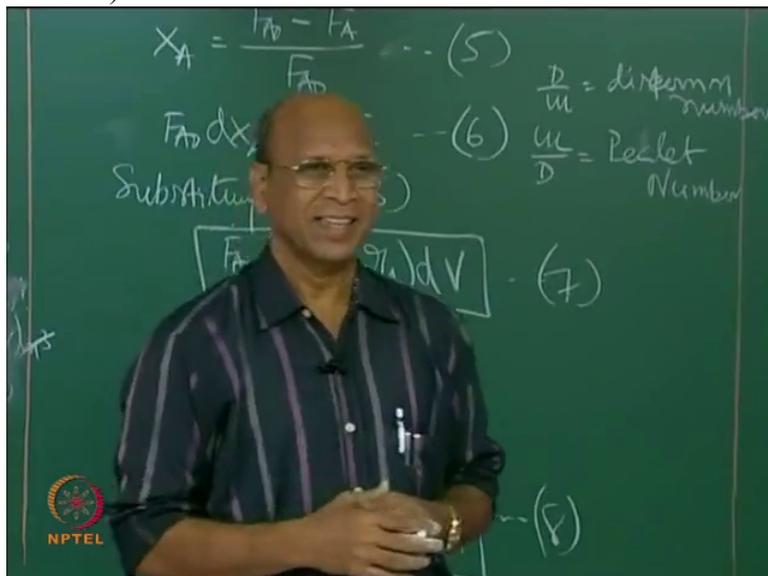
I have come with a lot of scent. Scent, spray, spray, Ok. Scent means you may not understand.

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Ok, That is old word, scent. Ok.

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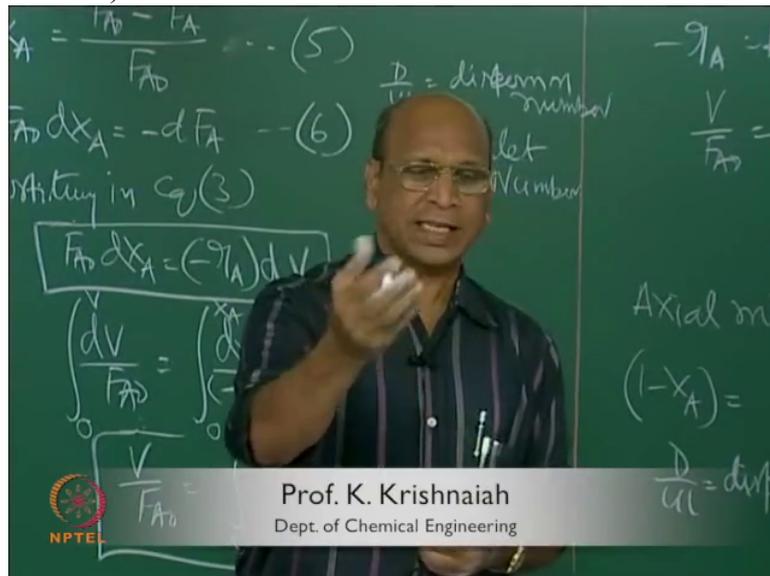


Yeah spray or deodorant, perfume, very good. Perfume and also by the way, perfumes are made by who?

Student: Chemical engineers

Professor: Chemical engineers. Yeah, all wonderful reactions, wonderful you know

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that is low volume high value product. Low volume, it will be 1 m m, 1 m l and 10000 Rupees. So there can you smell me?

Student: Yes

Professor: You have to imagine. I do not have right now spray.

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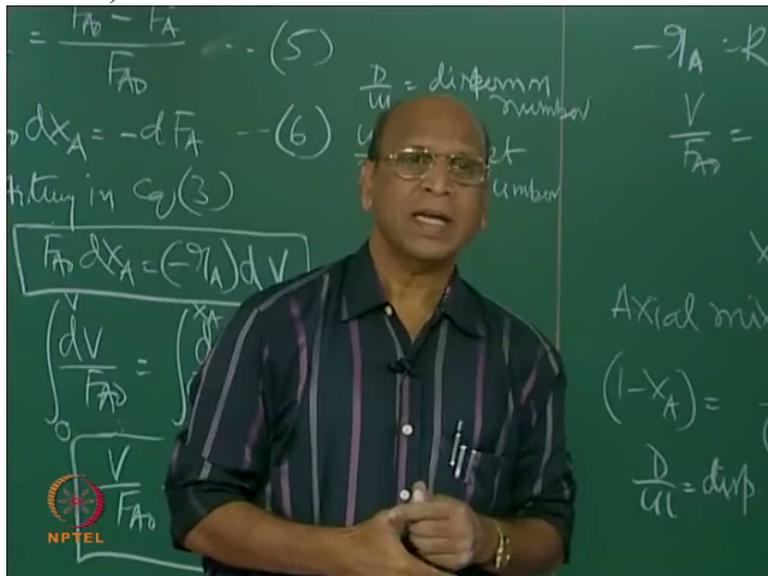
Ok. If I have all the perfume and then stay there, can you smell?

Student: No

Student: It depends on the chemical

Professor: Why no?

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Student: It will take time

Professor: It will take time. What is that time?

Student: Diffusion

Professor: Till then. I did not ask you instantaneously you know, smell. I did not tell that no?

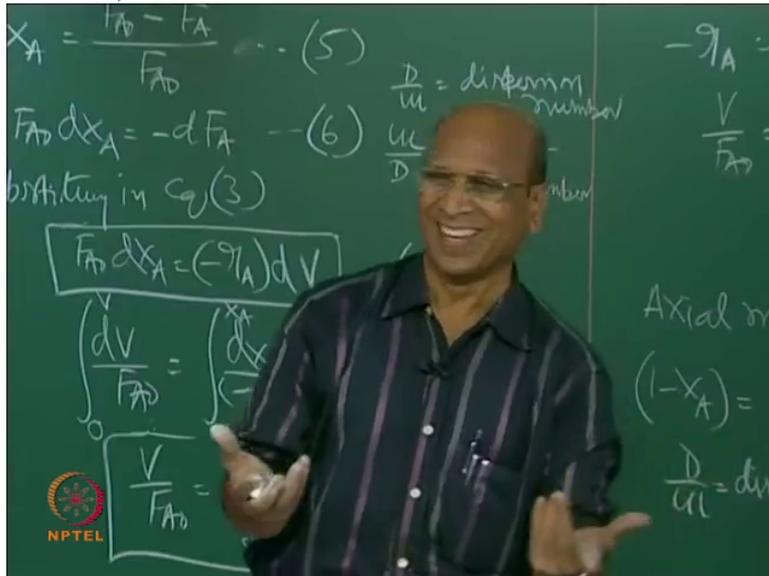
Instantaneously smelling also is there.

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(Professor - student conversation ends)

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Ok, the other example what I want to give is the conveyor belt. Many people are standing on the conveyor belt, that is the convection velocity, equivalent to, but some people enthusiastic, very enthusiastic people start walking on that. So that is by diffusion equivalent, right?

And you know what is the concentration difference, I mean what is the difference, the gradient for them because here is the concentration gradient, but for the people who are walking what must be the gradient? May be hurry. They have to catch the flight quickly. Or they have to move, you know, go quickly. So that is why those people are walking on the conveyor belt.

Other people are cool. Ok. Let it take me whatever time that is possible so they stand. That is by convection normal flow. Above that again you have diffusion. So now if you see Axon advertisement, you should not forget convection and diffusion. And also now, if you see conveyor belts, again convection and diffusion. But in ideal plug flow that diffusion is not allowed. In ideal plug flow that diffusion is not allowed, Ok.