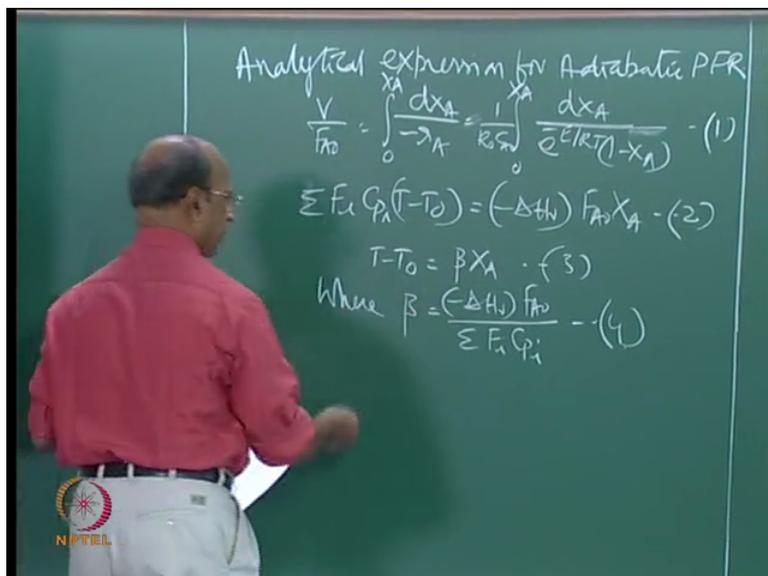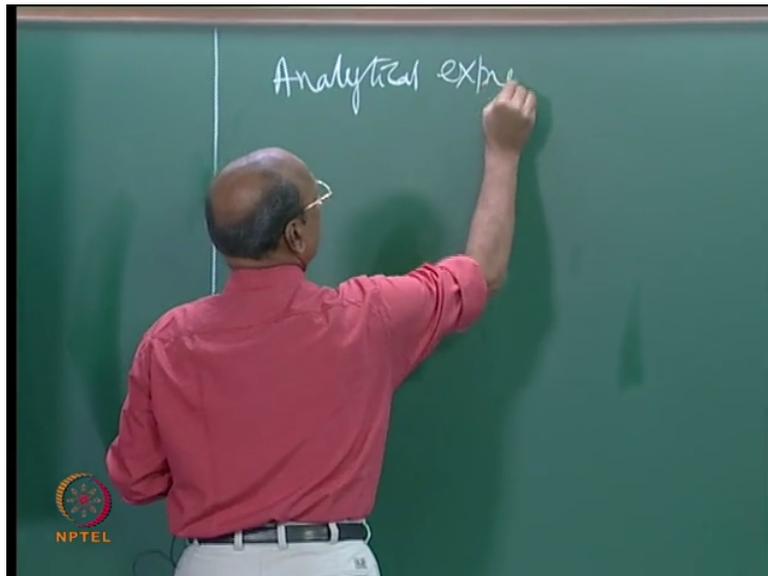**Chemical Reaction Engineering 1 (Homogeneous Reactors)**
Prof. K. Krishnaiah
Department of Chemical Engineering
Indian Institute of Technology Madras
Lecture No 46
Adiabatic Plug Flow Reactors

Okay, So this adiabatic analytical expression for.

(Refer Slide Time: 0:20)


Analytical expression for adiabatic PFR. Okay! So the equations which we know V by FA nought equal to 0 to XA dXA by minus RA which can also be written 0 to XA dXA yeah here I have to write K nought CA nought this may be already with you so this is E power minus E by RT 1 minus XA. Yeah this is equation 1 the other one you can remove of sometime.

I think why this equation I don't have tried this already you know that already you know. So V by yeah so the other energy balance equation what I have is sigma of FI CPA T minus T nought equal to minus delta HR into FA nought XA. Straight way after substituting you know that F nought XA I have written actually it is delta XA because XA not equal to 0 thats why I am simply writing XA there.

So that you will come in our format so T minus T nought is nothing but beta XA where beta equal to minus delta HR, FA nought by sigma of F of I CPI, yeah. So yeah I have to now substitute this T so this is equation 2, equation 3, equation 4, okay! So now substituting this T there because I have to convert this one in terms of, yeah here we are trying to convert in terms of T right?

Yeah for this analytical expression, otherwise we have to normally write this T in terms of X. Okay then integrate then you will have now all this you have now this entire integral we are now trying to convert in terms of T and of course limits also will be automatically in terms of T. So yeah V by FA nought I think. Yeah let me write this equation anyway.

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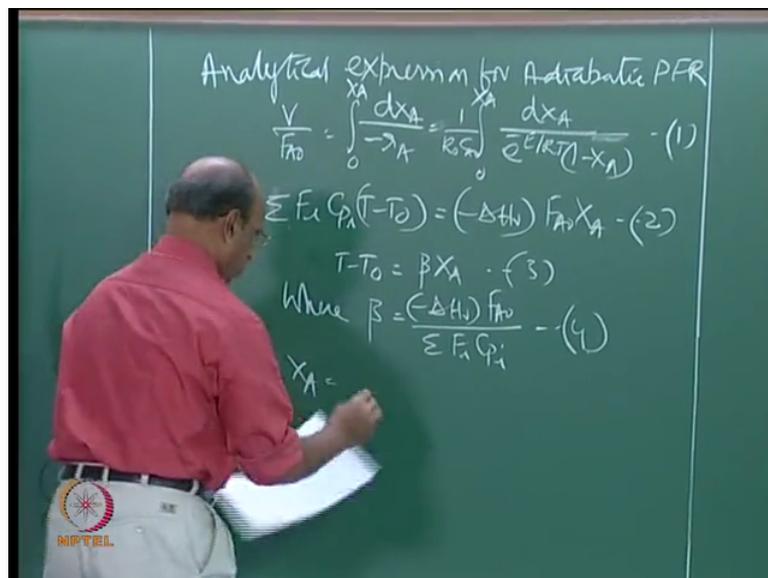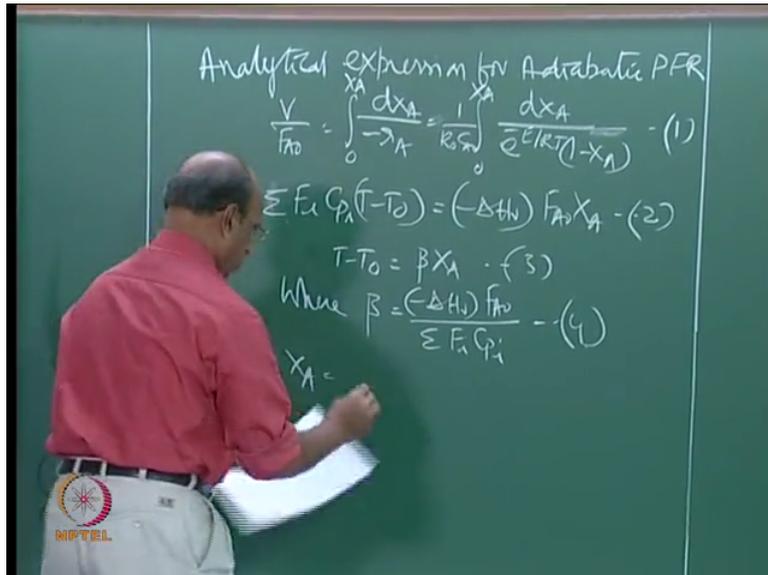
Yeah XA equal to T minus T nought, T minus T nought by beta which we also write this one as lambda T minus T nought. So this is equation 5 where lambda equal to 1 by beta where lambda is 1 by beta, yeah. Okay good, so now if I differentiate this equation then this will be dXA equal to lambda dT that is one expression. then I have to substitute this dT, dT will be in terms of okay dXA by lambda. Clear?

Okay good so then of course this from the same expression I can substitute for XA lambda T minus T nought and we and I am taking X nought is equal to 0. I mean XA nought is equal to 0. So in that derivation earlier which we have taken XA nought also was there I think I have not given that. Where lambda we given an equation no? Alfa, alfa equal to what?

Student: (())(4:40)

Prof: yeah lambda divided by
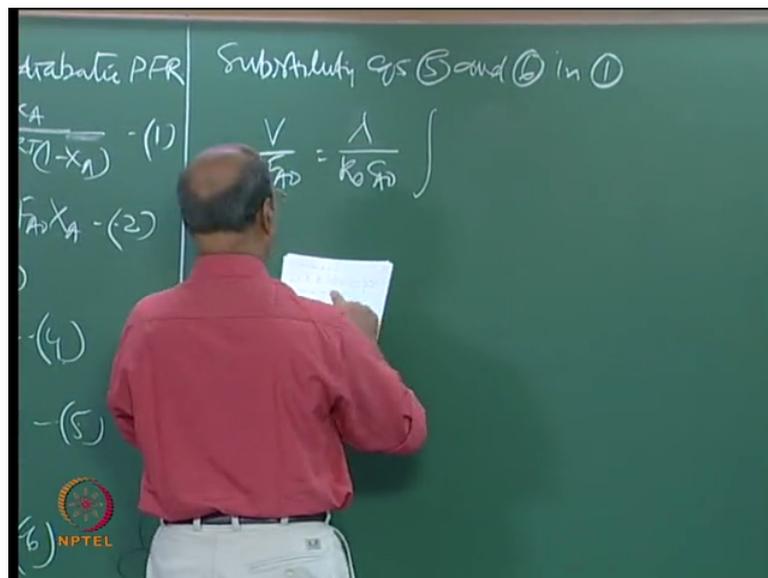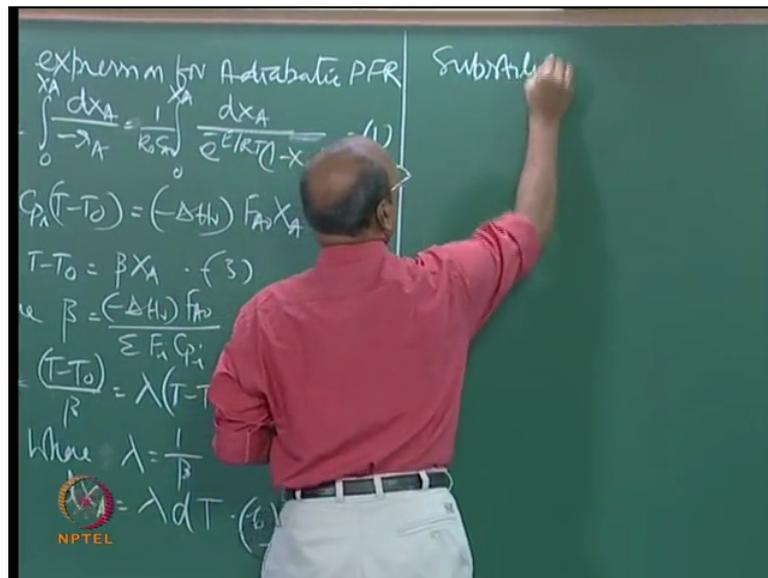
Student: I minus XA nought plus.

Prof: 1 minus

Student: IXA nought.

Prof: IXA nought that XA nought can be 0. That wont change the change in it, okay. So, yeah after substituting what I have to say is, substituting equation 5 and 6 in 1.

Substituting equation 5 and 6 in 1 only this one okay V by FA nought equal to yeah I am giving the final expression should have some gap here you have to quickly someone has to check this lambda by K nought CA nought integral E power U, okay I think in between I have to give I think another step. So that you will remember for continuity, okay.

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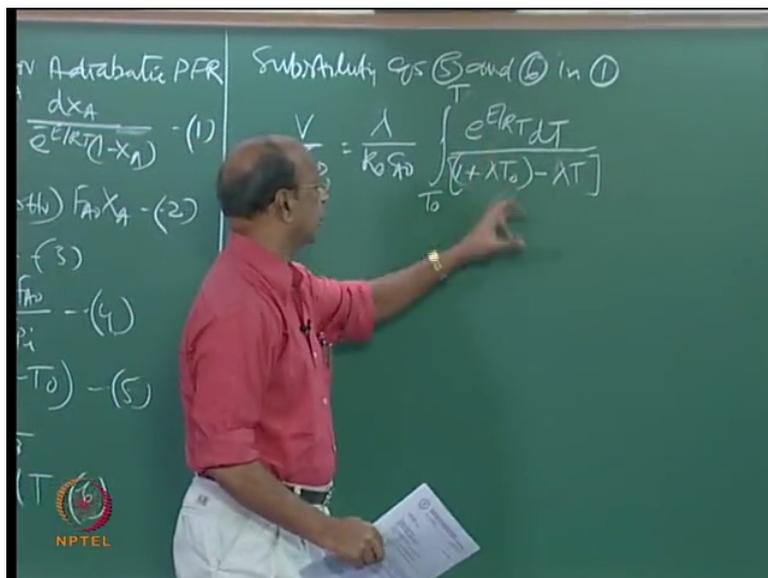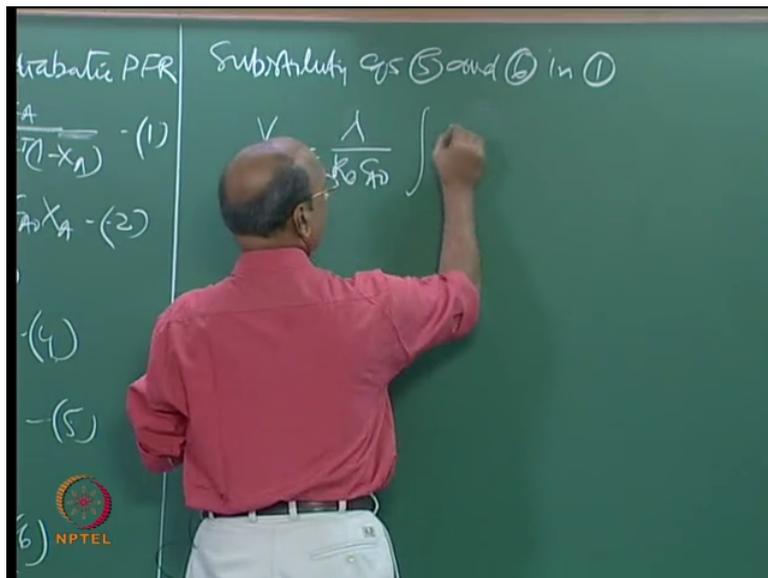
So this will be E power E by RT dT whole thing divided by 1 plus lambda T nought minus 1 sorry minus lambda T, please check this. Correct? Already so fast, correct? Yeah so now, if I1 go here XA equal to 0 fine. XA equal to 0 then I will have T equal to T nought because beta divided 0 nothing. T equal to T nought that is okay. But now final one in terms of T the XA equal to X means this equation only that equation is nothing but T equal to T nought plus beta XA, so instead of writing all that we have to only write this one here T nought.

Student: (())(4:40)

Prof: sorry T, you have to write T okay good. So now this yeah now there is another substitution which we have to do to convert this into that exponential integral because it is not easy to integrate. Okay and analytical expression we are saying its not correctly analytical

expression, it is still approximation because exponential integrate is an approximation they have tables where if you have that exponential of 1 may it go it may go to may be a point 22227 something like that and some value I am telling.

Okay so that is why it is still an approximation it is not the truly analytical expression the way we are imagining. Okay like for example our conversion X equal to for first order plug flow what is equation? For first plug flow? XA equal to? First order plug flow? First order plug flow?

Student: (())(8:09)

Prof: Yeah XA equal to 1 minus

Student: T power minus

Prof: T power minus (())(8:15) first order, okay. So that you have to remember correspondingly what is our batch and batch is almost same and for mixed flow these things minimum you have to remember. Okay yeah anytime so that what that is an exact analytical expression, right? XA equal to 1 minus E power minus KTOP it wont be like this. Okay like that equation but still it is an approximation but in terms of exponential integrals okay.

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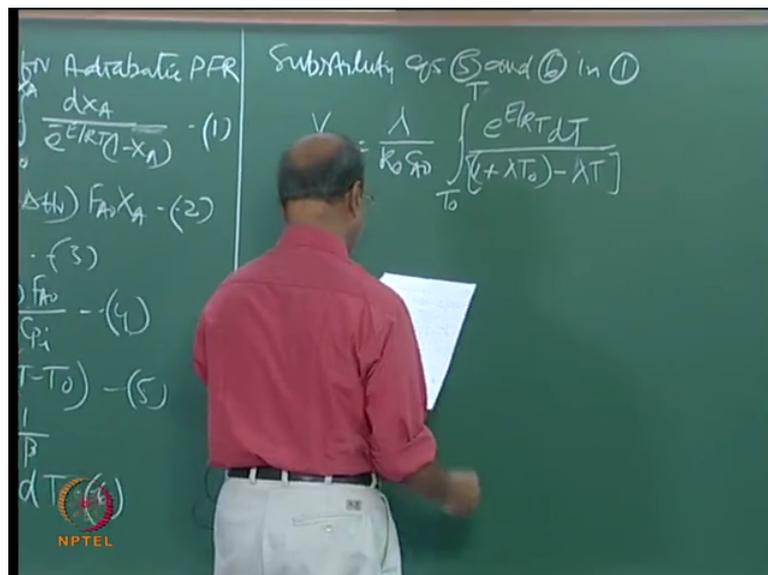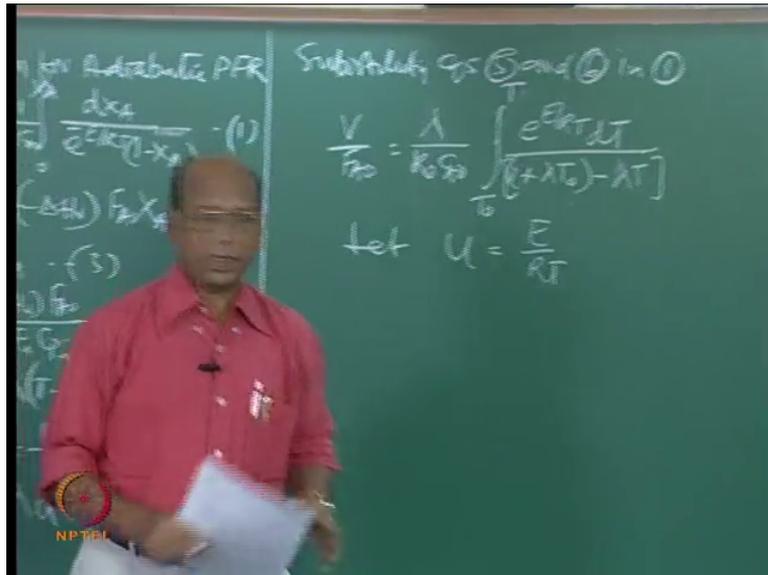
So now if I want to convert these to in terms of exponential integrals I have to now put another substitution U as E by RT because this E by RT as it is so this has to, why we have to put U if you don't like U you can put some other variable thats not the one, okay? Yeah why we have to write this one E that this one our exponential integral definition if you remember I think I would have given you that definition already, right?

Student: (())(9:19)

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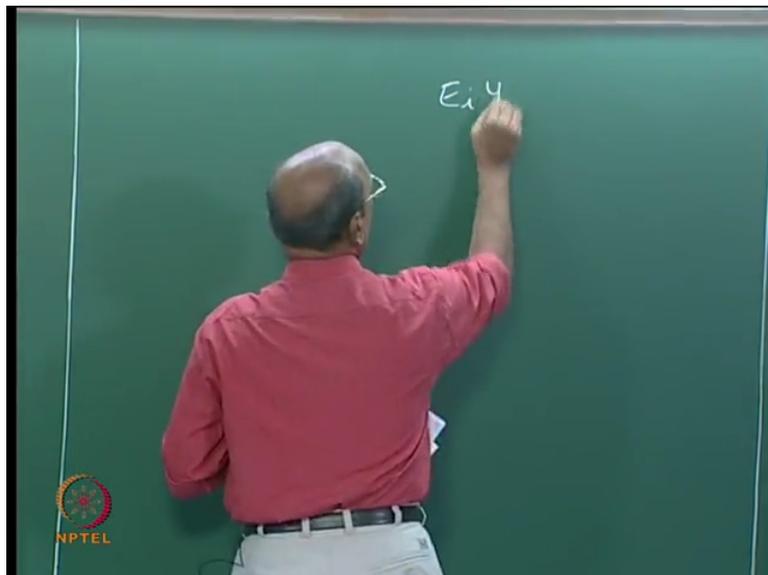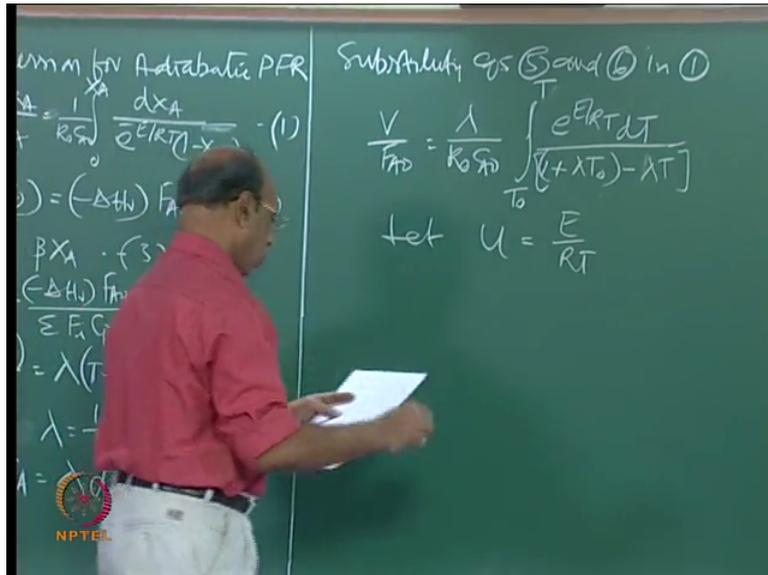
Exponential integral definition, I gave X or Y, yeah E of Y is minus infinity to
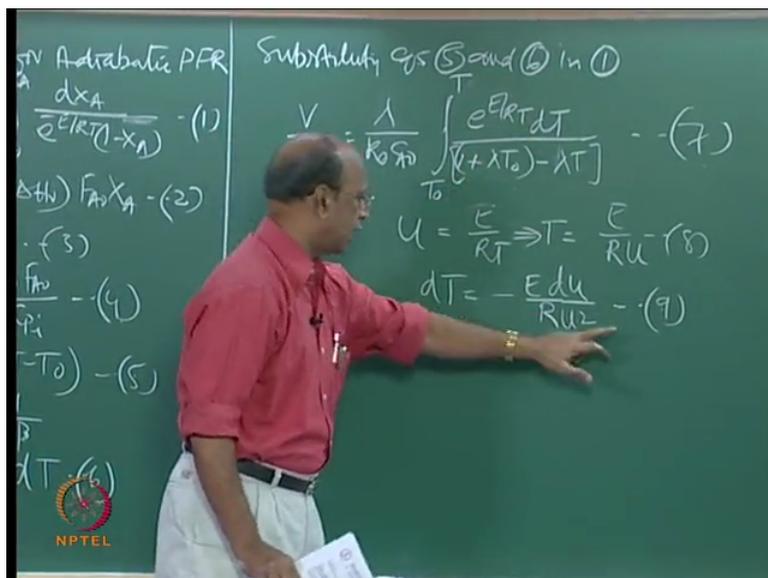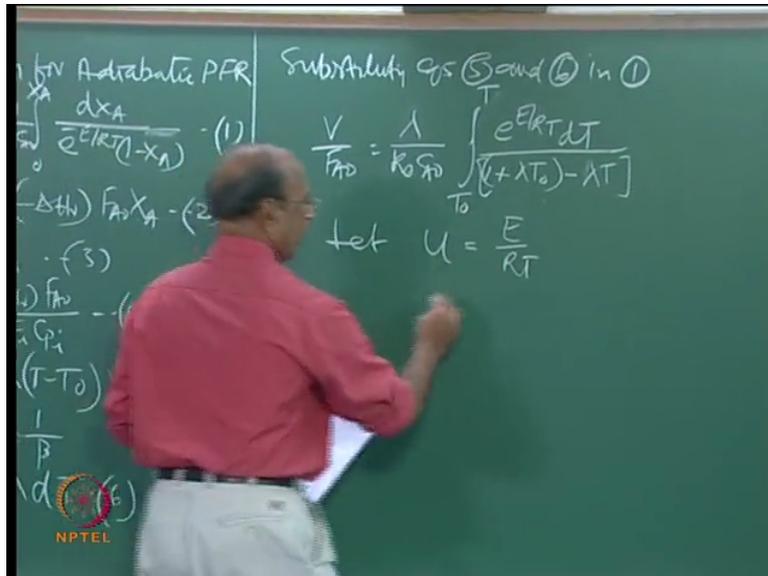
Student: Y

Prof: Y.

Student: (())(9:38) Sir T , dT.

Prof: Okay that is a dy variable I can write down E power T by T into dT so that is definition okay? So thats why I have to this is important for me. E power minus T by T form that is all you have to get and also the limits okay? Then only I can write this Ei and this Ei is listed in that (())(10:06) stogun hand book of nerimates or mathematical handbook okay?

Yeah so that is the book that is available. That is very famous book probably we have not used you know what till now. I saw that book only with professor Anand because I think he is PHD was highly mathematic, thermodynamics, you would have not know him because he was the director last year. you know him? You know because he is from your place. Acetate, he stayed in Acetate, came to Acetate many times yeah.

So only with him I have seen that book, I asked him sir where did you get this book we have not seen this at all. He said my, and also sometimes he has to use that you know exponential integral all kinds of our error functions. Error functions are also listed there. The values so for that calculation only I bought that one and then he was doing PHD in Florida long time back okay.

So this is the substitution because idea is to convert this into in that format, that is the reason why we are putting that.

(Refer Slide Time: 11:08)

So now we can yeah, we will write this equation. This equation 5 this is 7 yeah. So then U or T from this I can write as E by RU yeah. So why I have to write in terms of T is because this delta dT also have to convert into U yeah. Now tell me what is dT?

Student: (())(11:44)

Prof: Yeah dT.

Student: minus 1 by RT
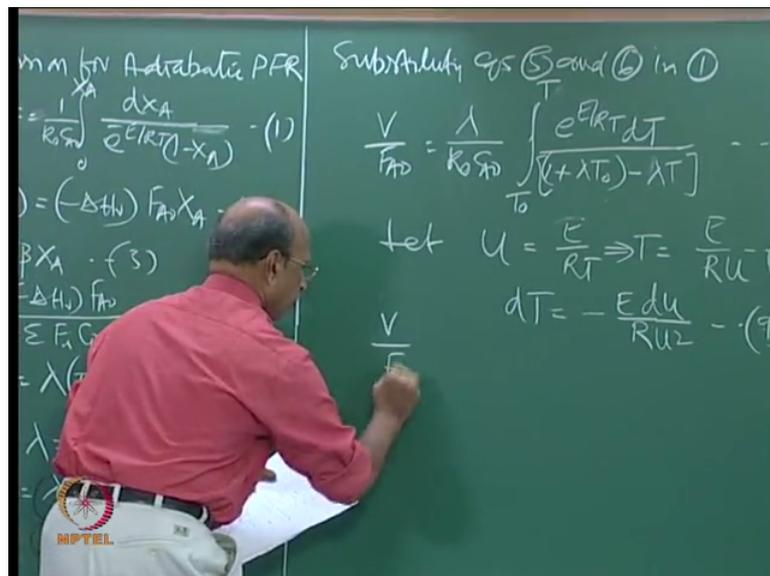
Prof: Miinus E

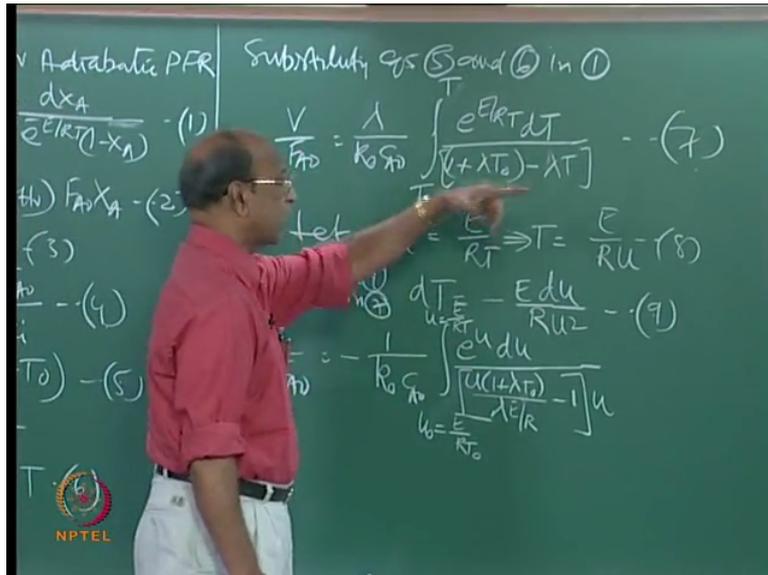Student: E by R

Prof: Yeah I write EdU by

Student: RU

Prof: RU square yeah. So that is the one what we have to substitute there that is equation number okay this is 8 this is 9 that is 1 and yeah.

So correspondingly for T and all I have to substitute this E by RU here, here only we have okay. So I think thats all with this substitution that means substituting equation 8 and 9, equation 8 because this T means here I have to substitute this one E by RU, right? This for this T and in 9 here I have to substitute 1 U will get cancelled right? Yeah here you take log take LCM and all that so here you have U square. And here you have U in the denominator so that U will get cancelled and the final expression what you get is.

(Refer Slide Time: 12:56)

Board content (left panel):

Adiabatic PFR

$$\frac{dx_A}{e^{E/RT}(1-x_A)} \quad (1)$$

$F_{A0}\,x_A \quad (2)$

$\quad (3)$

$\quad (4)$

$T_0) \quad (5)$

Board content (right panel):

Substituting eqs ⑤ and ⑥ in ①

$$\frac{V}{F_{A0}} = \frac{\lambda}{k_0\,C_{A0}} \int_{T_0}^{T} \frac{e^{E/RT}\,dT}{(1+\lambda T_0)-\lambda T} \quad (7)$$

$$let \quad = \frac{E}{RT} \Rightarrow T = \frac{E}{RU} \quad (8)$$

$$dT = -\frac{E\,du}{RU^2} \quad (9)$$

$$= -\frac{1}{k_0\,C_{A0}} \int \frac{e^u\,du}{\left[\frac{u(1+\lambda T_0)}{\lambda E/R}-1\right]u}$$

$$u_0 = \frac{E}{RT_0}$$

Yeah V by FA nought equal to again I have to write substituting equations 8 and 9 in 7, in 7. Yeah V by FA nought equal to minus 1 by k nought CA nought integral E by U dU, 1 plus lambda nought lambda T nought by lambda E by R thats correct only, yeah minus 1 this again whole thing multiplied by U yeah. Now the limits here again you have to go to this one okay?

Yeah so this will be when T equal to T nought this will be U nought so thats why what we write here is U nought which is nothing but E by RT nought similarly in the here U equal to thats all E by RT, thats all. Okay? Yeah, so there is another again substitution that will come to convert exactly into this kind of exponential integrals. Okay I mean because I am taking lot of time I say.
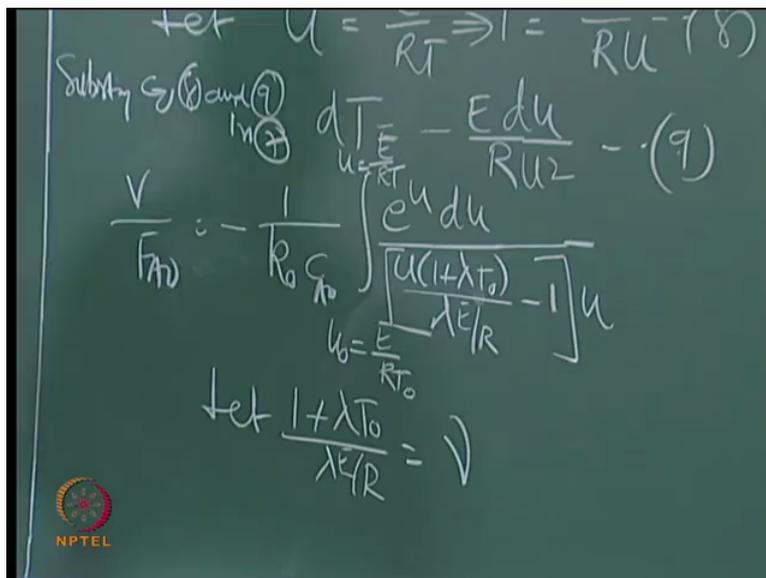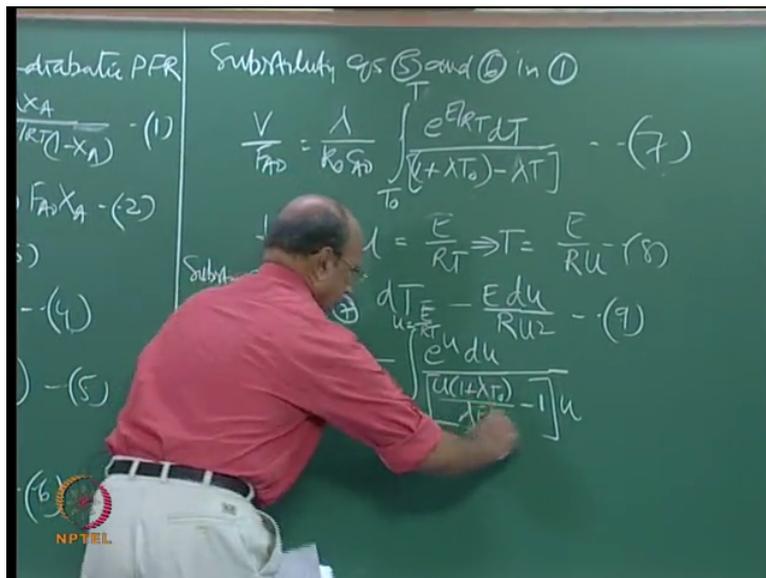
Yeah so another one I think for easy remembrance this entire thing let my god my time was gone whole 1 plus lambda T nought by lambda E by R what I substitute was mu. So now this equation will be simple equation.
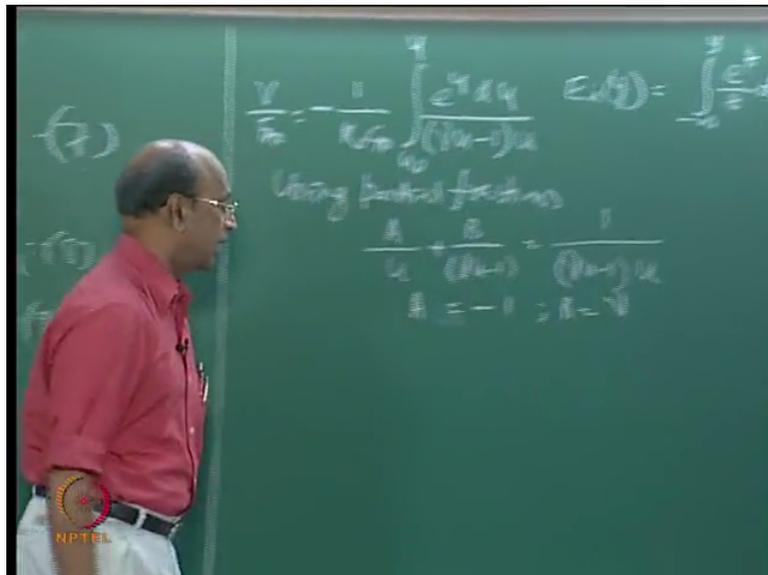
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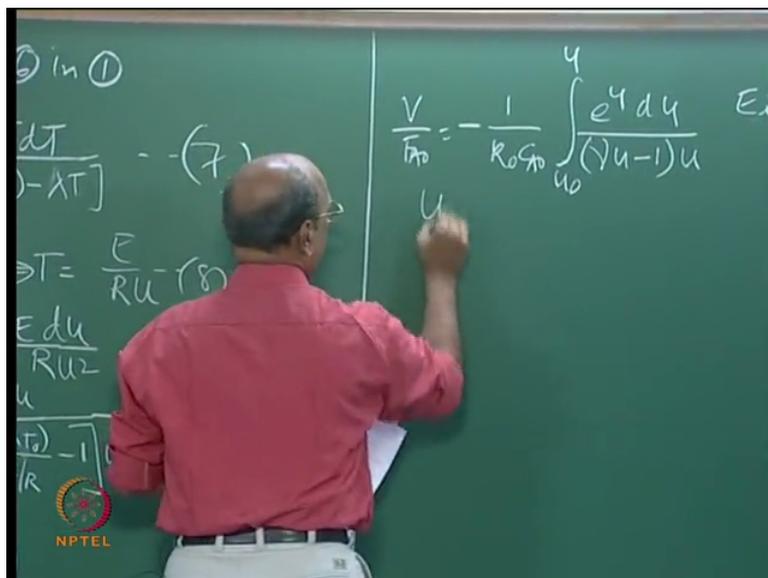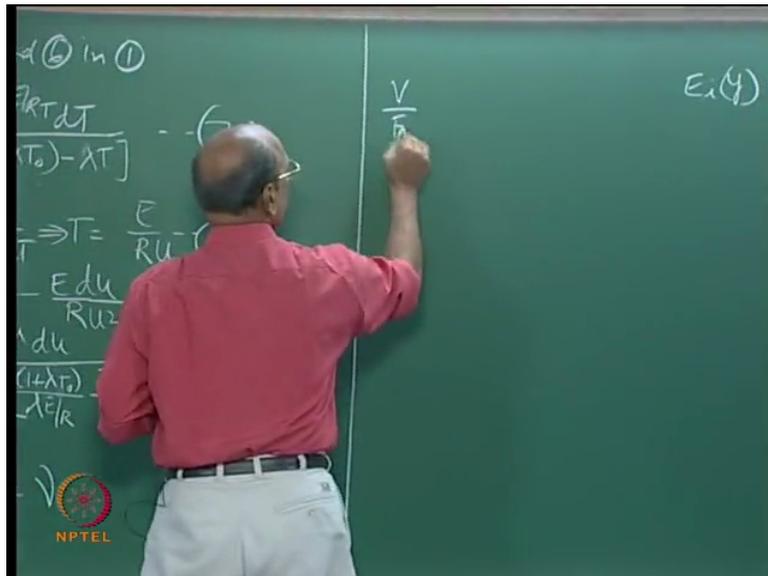
Like V FA nought equal to minus that minus is there 1 by K nought CA nought integral U nought to U, U plus lambda U not lambda this is mu, mu U minus 1 that is. Correct? Check? Yeah so now how do I integrate that one.

Student: (())(16:24)

So you have to that split into partial fractions okay? So when you write that partial fractions I am solving the whole thing now almost, okay let me write that partial fractions.

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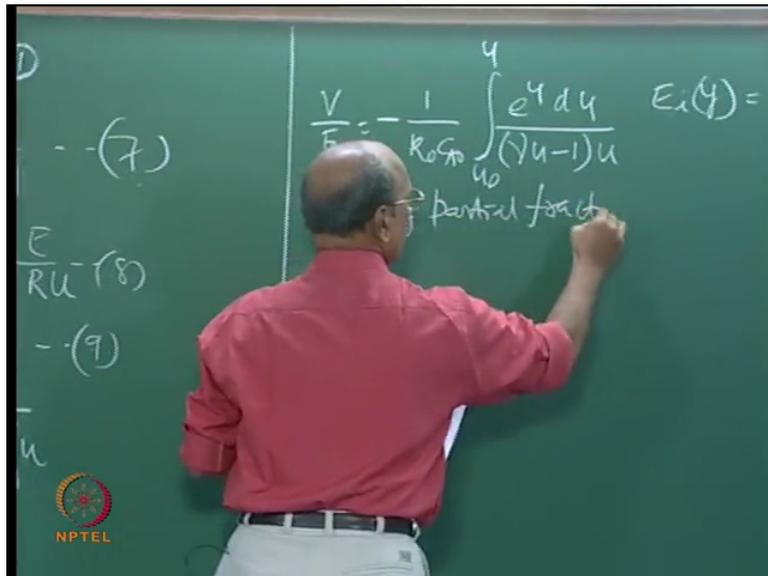
So now using using partial fractions we have A by U plus B by mu minus 1. These are we write now, yeah now tell me what is A and B?

Student: This is (())(17:15)

Prof: (())(17:15) answers? A is minus 1, B is mu right correct. Okay

(Refer Slide Time: 17:22)

So now I have to now split this into 2. What swami last? This why this is the reason now its all mathematic class, we have forgotten about what we have done. Beyond this, beyond this after energy and material balance okay, now it is only solution, solution, solution there. Substitution to get another thing another substitution to get another substitution like that it has to go.

Okay but anyway these things also are required for definitely that higher level when you go to slowly deeper and deeper into subject you cannot avoid mathematic. And you should not avoid that. But all of us have this phobia for mathematic because we have not in touch with mathematic. Thats why, if you are in touch with mathematic you will not afraid.

Right I could have not made that mistake of you know writing that limit, only thing is we are not in touch with that so we will forget sometimes, not sometimes many times you forget. Okay good.

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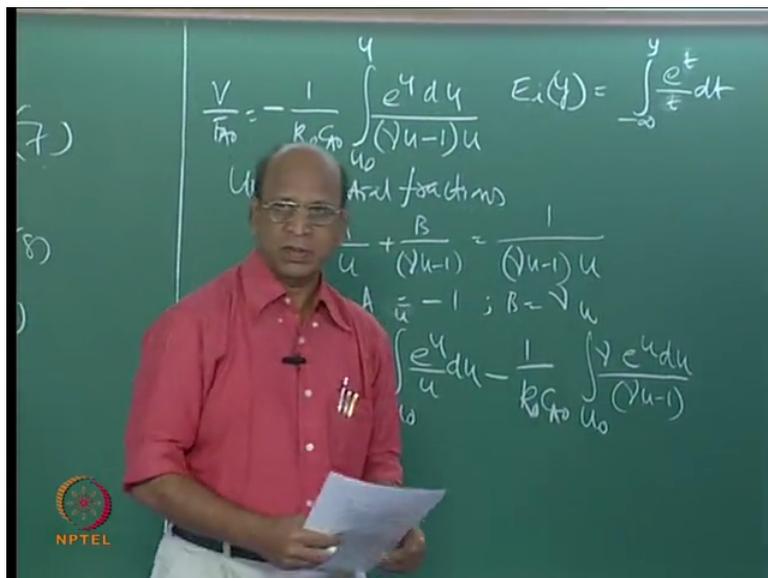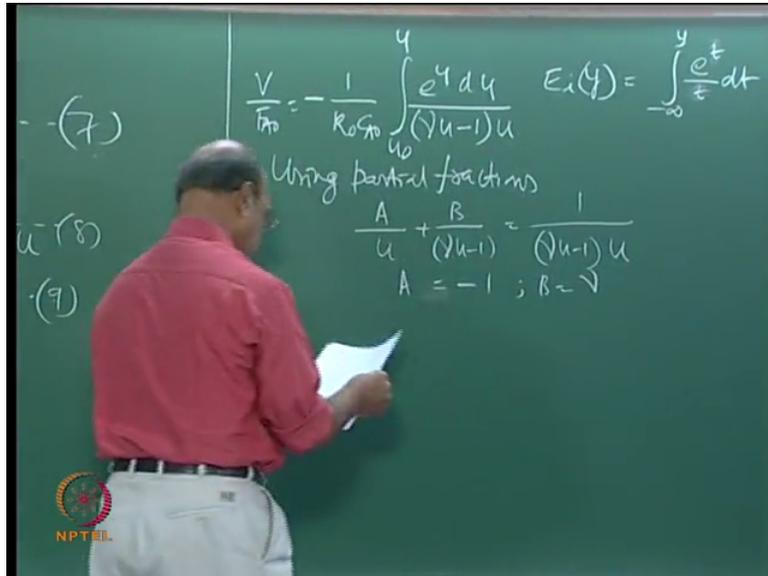
So once I do this substitution the expression what I get here is V by FA nought equal to 1 by K nought CA nought this U nought to U then E by dU that is 1 fraction, then I have another one minus 1 by K nought CA nought. My handwriting I think this chalk is spoiling my handwriting, otherwise it not that bad. Okay 1 by K nought CA nought again U nought to U mu E by U into dU minus 1 so this 2 okay.

So here what I can do is again divide my god whole thing I have to write this I will divide by mu so this becomes U minus 1 by mu. Okay so I think I will write that one directly hopefully you don't mind?

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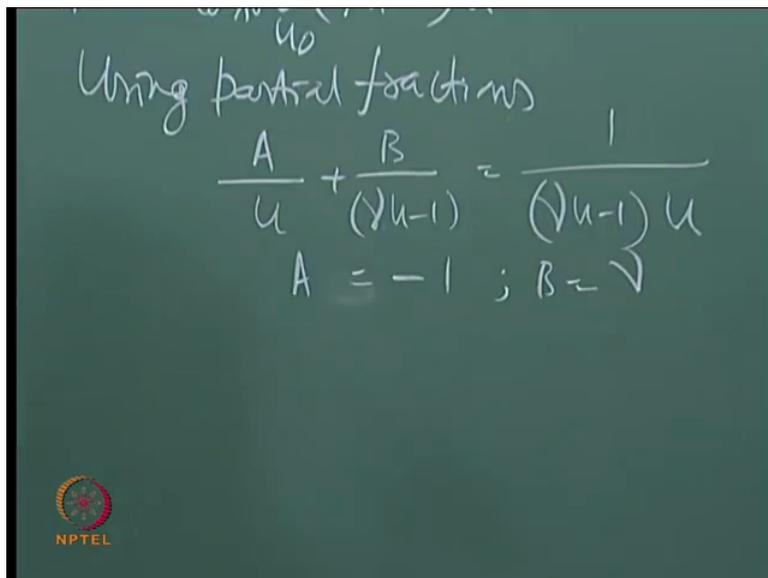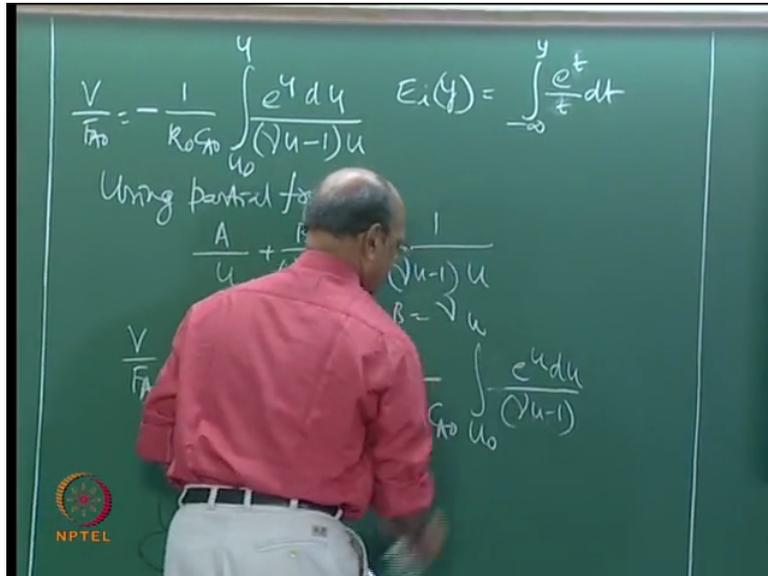
So this is U minus 1 by mu. Okay you have the equation for mu. Mu is this, I lost naming this okay. So this is 10, 11, 12, 13, 14 okay. So here mu values I know mu is nothing but this. This one 1 by lambda 1 plus lambda T nought by this one okay. So there is another substitution where you have to make that substitution that is Z, capital Z equal to U minus alpha where alpha equal to 1 by mu, okay?

Yeah this one where alpha equal to 1 by mu also equal to lambda E by R1 plus lambda T nought, yeah correct? This what we have also written lambda alpha value. Okay? Good so
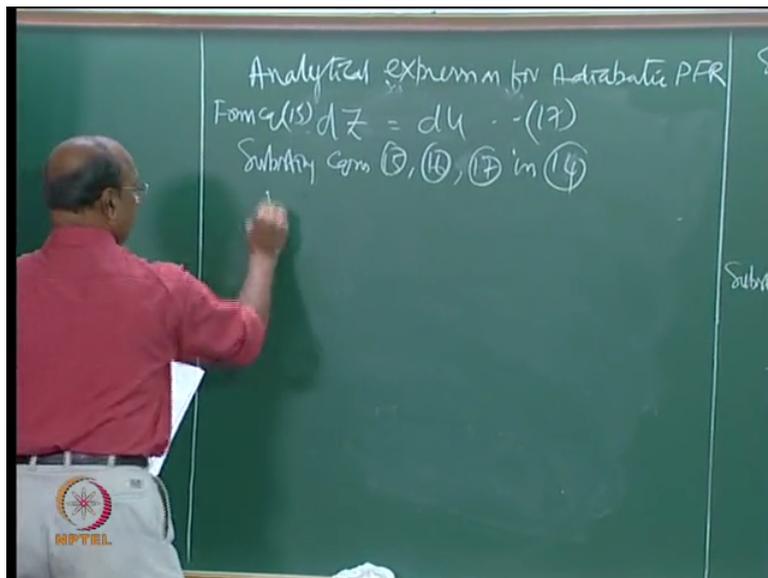
this is the one, so now again using this I have to convert this limits as well as you know into exactly this is no problem for me. But this I have to again convert that. So by putting Z equal to U minus alpha what is I am trying to do now?
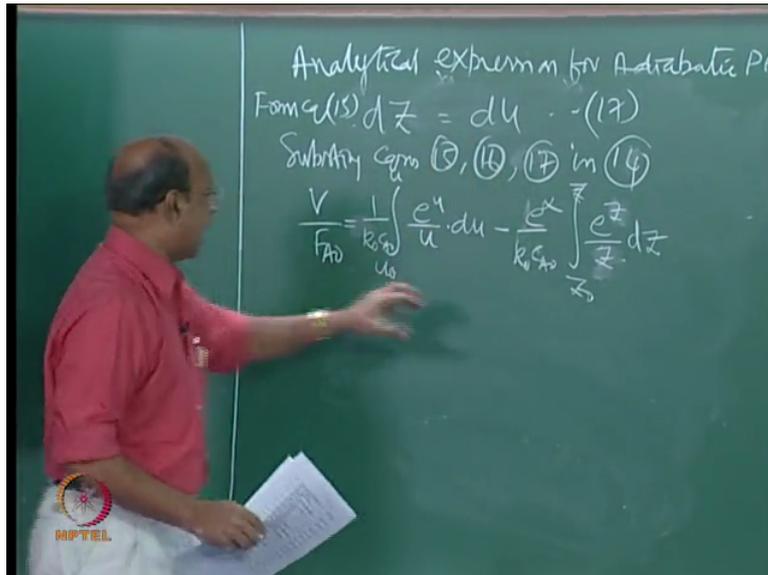
U equal to Z plus alpha, right? So here I will have E power Z plus, plus alpha so that means E power alpha is a constant, correct? That I don't have to integrate this all this thing I know, alpha is a constant that will come out, right? And then you have this entire thing anywhere Z, right? So E power Z by Z into dZ you know this yeah, okay what is dZ here?

dU so there is nothing so thats why its entire thing will become now E power Z by Z and you have here E power alpha which is constant which I can take out. Okay? And limits also there is no problem that directly becomes Z zero and this will becomes Z. This will become Z zero and this will become Z. So then I will have the exponential integral, thats all I think anyway let me, let me do lot of only giving few steps but ended up giving up the entire thing (()) (22:51).

Okay these equation numbers I have to put this is equation 15, this is 16, and also we have another equation dZ equal to dU this is from equation, okay from equation 15, okay so now substituting equations yeah 15 and yeah 15, 16 and 17 in 14. Substituting equations 15, 16, 17 in 15 in 14 yeah cannot write that okay.

(Refer Slide Time: 24:02)

Analytical extremm for Adiabatic P?

From q(15) $d\bar{Z} = dU$ ...(17)

Substituting eqms ⑬, ⑭, ⑰ in ⑭

$$\frac{V}{F_{A0}} = \frac{1}{k_0 C_{A0}} \int_{U_0} \frac{e^U}{U} \cdot dU - \frac{k^\alpha}{k_0 C_{A0}} \int_{\bar{Z}_0}^{\bar{Z}} \frac{e^{\bar{Z}}}{\bar{Z}} d\bar{Z}$$

So what you get is this expression V by FA nought equal to yeah anyway this tail is there always k nought CA nought so this will be U nought, this will be U E power U dU minus again 1 by K nought, CA nought yeah so this will be Z0, Z yeah E power alpha I will take out here E power Z by I think I am writing capitals dZ right? But still the problem is that we don't have here that exponential, this is minus which minus you are talking?

Limits okay that minus infinity how do I do that here?

Student: (())(25:18)

Prof: If I can split this is U 0 to minus infinity and minus infinity to U, you can split now in between right? So thats all if you write this one again as splitting yeah minus infinity to U nought sorry U nought to minus infinity and plus minus infinity to U and this one you can write as minus, minus infinity to U nought so everything is in place similarly there also that is how you got that final expression.

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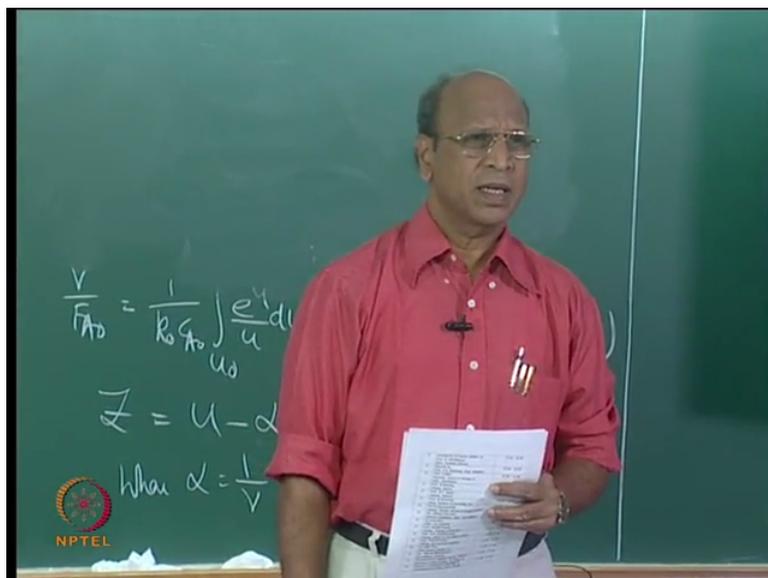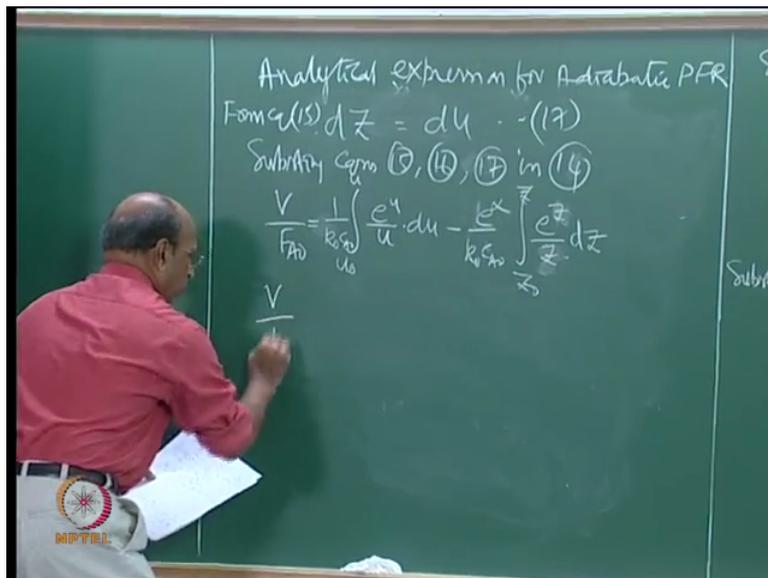
Okay V by FA nought equal to after splitting that okay, and substituting the corresponding things. K nought, CA nought exponential of E by RT, minus exponential of E by RT nought, okay this is one minus okay minus E power. I will write here minus okay E power alpha by K nought CA nought and this bracket I bring here yeah this is the Ei of Z minus Ei of Z0 so that is the one way to final one.

Okay so this is here and the exponential integral, I know some of you would have been definitely switched off your brain okay this is what happens when you talk only about mathematics in the class. After sometime 50 percent, 60 percent then 70 percent finally 100 percent after sometime, okay. Like this you know every class is there with lot of mathematic

because, somehow we know we don't enjoy doing mathematic that is our problem if you are able to enjoy mathematic.

And you cannot avoid as engineers you have to definitely enjoy mathematic. Somehow you don't have that practice I am going frankly you just imagine, I think all of us would have taken particularly we I think 5 year course we have taken maths 6, M1, M2, M3, M4, M5,M6 how many you have taken.

Student: 6, M6

Prof: For your its M6 so mathematic portions are not reduced.

Student: Sir M4.

Prof: For you M4? 3 years 4 years?

Student: 4 years.

Prof: 4 years where? Which place?.

Student: Government engineering Calicut kerala.

Prof: Calicut government engineering, okay. So that is why even though we have done so many courses in mathematics but still we don't enjoy? Why Rashmi?

Student: Understand mathematics.

Prof: You enjoy? I am not talking about you. You generalise the answer you don't know? Yeah anyway that is the problem okay.

Student: (())(28:33)there teaching is (())(28:38)

Prof: Yeah may be that is also required particularly when you the real mathematic course they don't have to connect. Real M1, M2, M4, M5, they don't have to connect but later somehow that is why we have you know what is called chemical engineering mathematic there that connection. Like that everyone I think I don't know whether civil engineering is have mathematic, are you absent? Okay

So may be last class I think everyone is absent that one mathematics discussion, okay. So like that I think after sometime only 2, 3 people only Rashmi wil be there after sometime. So this

is the problem you know thats why I always I try to talk more about physics more about how did you get the equation rather than the solution.

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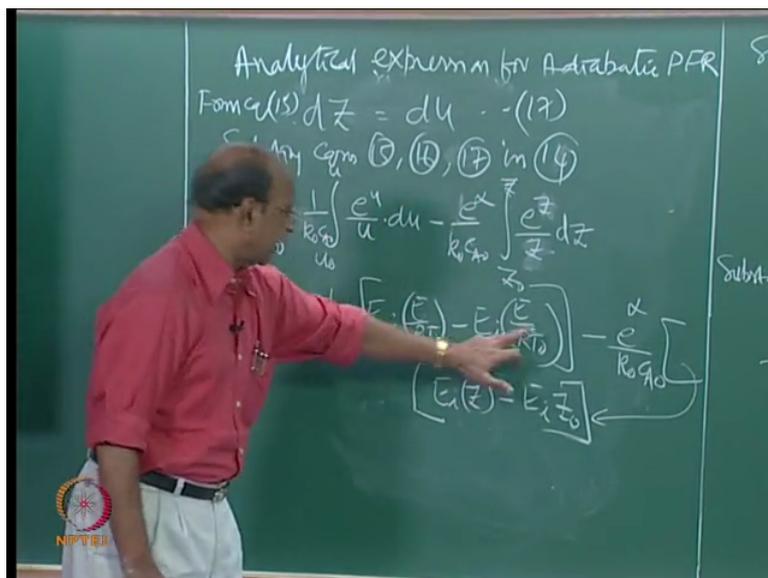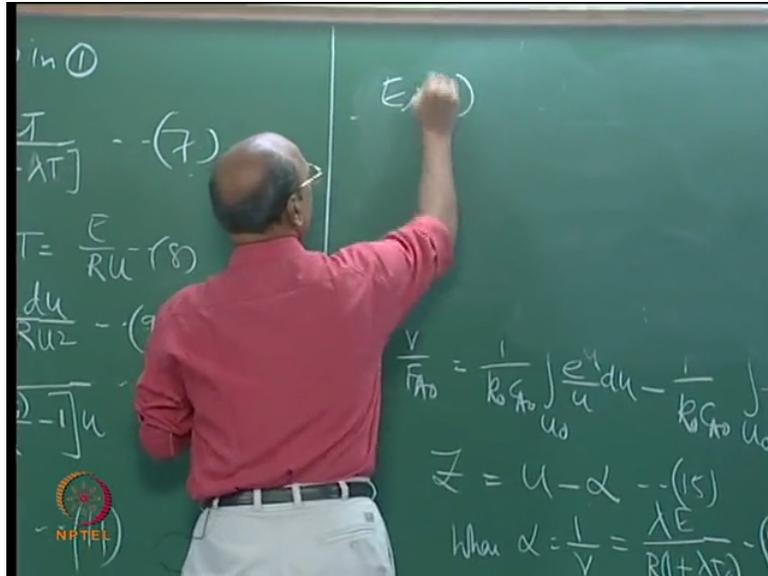
Okay so this minus infinity to Y, E power T by T dT these also you know approximation not a (()) (29:35) this is point 57722 plus lon Y plus Y plus Y square by 2 and 2 factorial plus Y cube it is nice beautiful symmetry in all these things. 3, 3 factorial plus goes on for the solution. So if I say that Y equal to 1 what is the value? You can calculate, right? If I have two 1.5 or 1.1 whatever even 1.1, 1.2 whatever right?

Yeah but in this case our value is E by RT, right? Our value is E by RT so E by RT you know equation but be careful about the units particularly you cannot use calorie CR and here you cannot use joules, all okay? So that is why you and T is always in Kelvin all those problem

will be there so for example if value is 2.2 then you can go there and calculate what is this. Similarly this, similarly this, similarly this then you will get that. Yeah there is another also definition of.

(Refer Slide Time: 30:57)

This is noted as small I, small ei, this is also called exponential integral, right? But the definition of this is yeah definition of this is X to infinity, X to infinity this is E power minus U by U dU this also has this expansion this is same thing what minus 7722 minus lon Y plus Y minus Y square by 2 factorial now plus Y cube 3, 3 factorial minus this is Y. Okay write write.

So that is what you know actually these things in the latest book of (())(32:07) he has included this. I don't know whether you have seen that or not. Latest books means I am the third edition what you have, you are not born when the second edition came. But third edition

is the one which most of you are using and I don't know how many of you have read RTD chapter it is an RTD chapter it also comes in (())(32:28) there is one equation I again which you cannot solve you cannot have analytical solution so you have to go for exponential integral.

Okay in some place you have to go to error functions. Right? So thats why I told you know please remember all my words they all are beautiful words not only in the class I think even after in life also okay. Beyond certain points CRE is nothing but mathematic. But unless you reach that point you don't enjoy mathematic, okay.

Yeah those who enjoy mathematic there are 2 books I think Aries is one the other one also who went very deep into mathematic is Froment bischoff. I have written sometime back I think last class Froment bischoff of chemical reactor analysis and design I think 79 or so 1979 but your question mark I don't know exactly, right but there are 2, 79 second edition also has come first edition I think is in 1979 second edition may be 1992.

Okay but I think you also should know the idea of any course is you have to expose more beautiful things and also you have to learn basic. That is the idea of any course, right? Its not that always only basics but basic plus exposure to complicated things this is one of the exposure to complicated things. Right those 2 books are very very deep I told you know we are loosing you because unfortunately in our university.

And colleges I think it is not that much you know there are 2 courses I think that much rigor rigorous training in CRE is not there. Sorry to say this because last 10, 15 years I am conducting that 0 examination okay that 0 ethic test. And I have shown you know most of the time it is only empty yeah out of 30 all those 30 questions are wonderful questions.

I have not asked mathematic number 1, I just asked only simple question like of course everyone knows only what is heterogeneous system, homogeneous system and other one is, what is the other one? I told also.

Student: Elementry

Prof: Elementary, logmentry also many people don't know. Another thing is only differential and only 2 actually there are another 2, 3 okay yeah half life method is there. And linear regration is there ideally it is many people don't know, yeah differential analysis and integral analysis thats what only we have done, they have given. Only these two questions almost

every one answers but again you know even the other reactor there they write MFR, CSTR, BMR and batch reactor. Plug flow they have forgotton all three are same only correct?

Some people called mixed flow reactor, some people called continuous stir tank reactor, some people old people called batch mixer reactor if one of the oldest process I still teaching in your university then he may call it only batch mix reactor. Okay so all those 3 that is why that also not mean any benefit. May be percentage wise slightly better than other places so if that base is there.

And if you are excellent before I ask question you are answering in basic so then I think we could have gone to this and this highly mathematic okay. So that is what is unfortunate thing that is happening last so many years thats why I thought after my retirement I have to go to I have to train the teachers that is one of the aim I thought in my mind. You may they have to call me I cannot go on my own because so I don't have that much money to travel and go.

Okay I will now teach you no one will come also. Okay so thats why I thought you know teacher should be train first in CRE then something may happen okay. I think of the overall picture I told you there is our beautiful quotation that we teacher not only teachers we gives an attitude towards the subject and there is another also I think sometime back also I told in my room it is there always right?

I think that that is more important than simply solving problems like this approach to it. Okay okay an approach to it and also an attitude toward the subject so that means after taking that subject automatically your attitude toward that subject should change. Your approach should change okay approach I have already mention in CRE the beautiful approach is you should know only kinetics and you should know only contact not (())(37:20)

Contacting thats all what you have and you know approach is the subject only not only you not day to day solving of the problem yeah. So that is why I have been telling you once you learnt that 3 contacting patterns batch and continuous too you don't have thats what I have been telling you. You don't have to anything more to learn if you are train to address only ideal contacting and I tell you 99 percent of the time you go only for ideal contacting then what is left now?

What is left is only kinetics and kinetics are very very trouble solve. Very very complicated I can tell you, right? Because first of all you don't know if I write okay. Abdul what is the order of this reaction.

Student: Dont know sir.

Prof: Yeah really Abdul don't know or order (())(38:25) we don't know. Order you don't know yeah so we cannot simply take get any information as A going to R. Okay absolutely we don't have any idea but on the other hand I write this equation.

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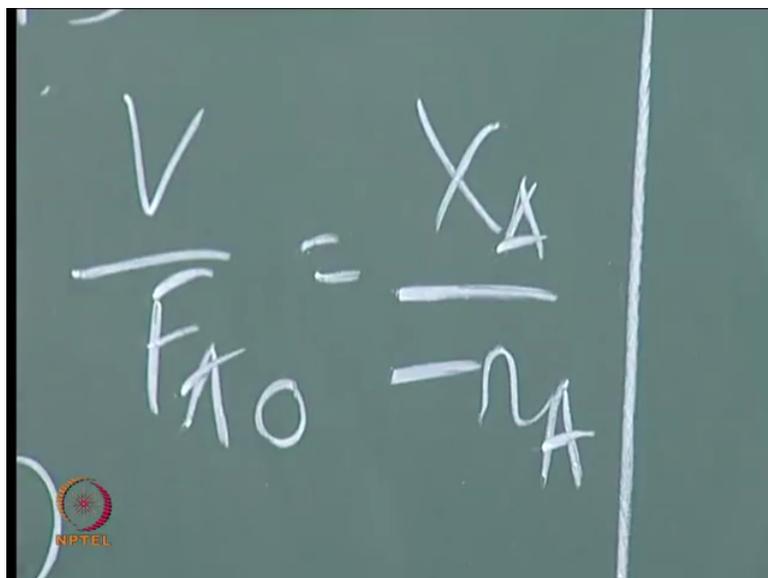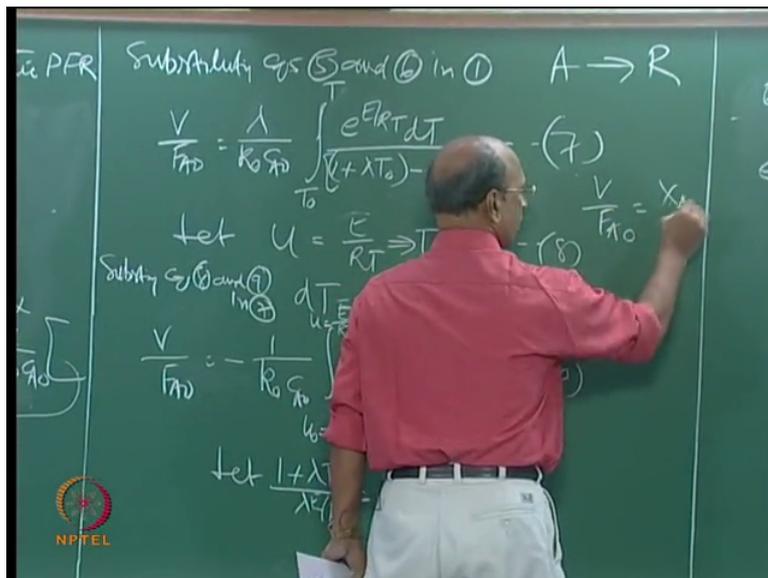
Yeah what is this represent?

Student: CSTRE

Prof: Are you a kinetics this also very simply question. I know the kinetics so similarly I can write for batch and can also write for plug flow. So the moment I look I know what is happening there, yes that equation I get only when I have mixed flow. No equation no other contact department will give you like this. That is why the here contacting is much easier because the moment look at the equation then R even the equipment.

You know right most of the time it is a tank where you put this stir and all that okay this must be CSTR if there is input and output. If there is no input and output only continuous stirring and all that we should have batch. The other one always 2 lines for plug flow in a pipe so that is why you know much more information for in contacting then kinetics absolutely kinetic you don't know anyway next time particularly when you come to catalytic reaction and also non catalytic reaction in a heterogeneous system.

You don't have any idea about what kind of reaction it is that is why all our approach should be how to solve this kinetic, okay? That attitude is liking that once I have this kind of clarity automatically my attitude changes. This subject is very easy. Why its very easy? I should no only 2 things, one is contacting other one is kinetic thats why my attitude is very simple thats all what I have no complication.

But when you go to kinetics in go to deeper and deeper you will have more and more problems in the in getting the kinetic, okay good we will stop now because I don't want to start now that mixed flow reactor so thats why I spent this time.