**Chemical Reaction Engineering 2 (Heterogeneous Reactors)**
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**Module 01**
**Lecture 33**
**Design equations for Packed bed reactor design**

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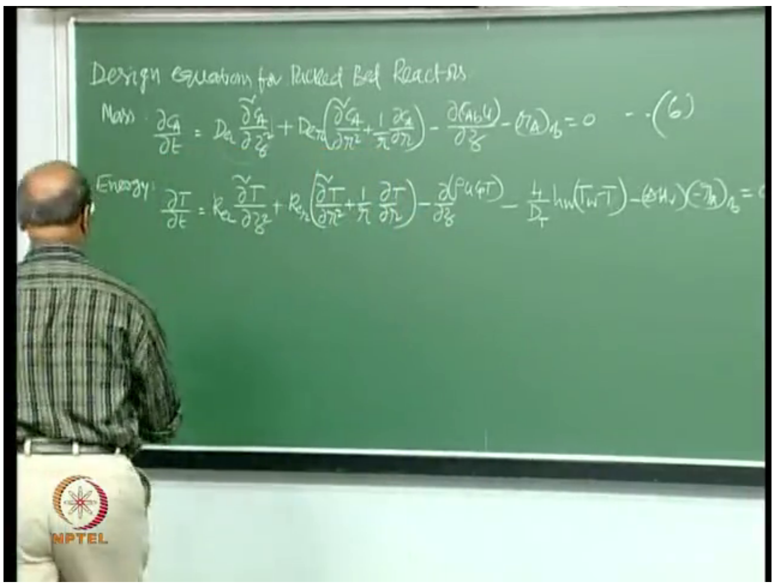


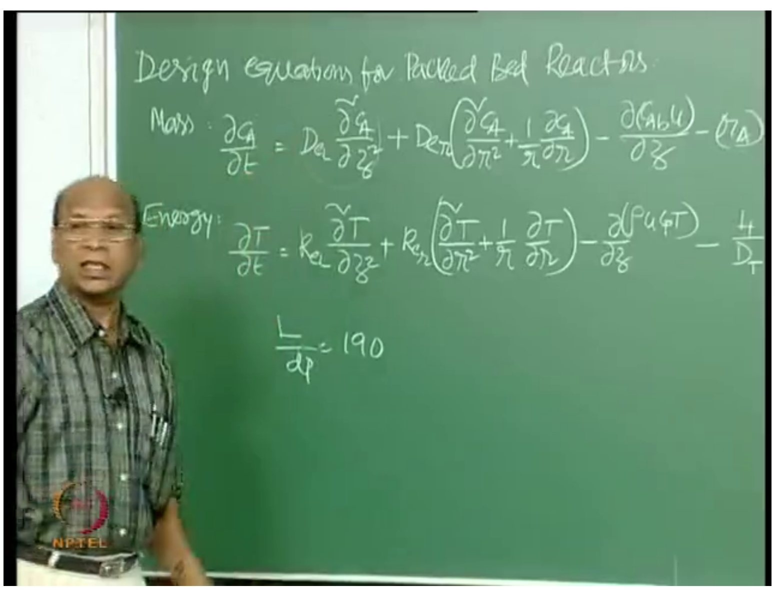

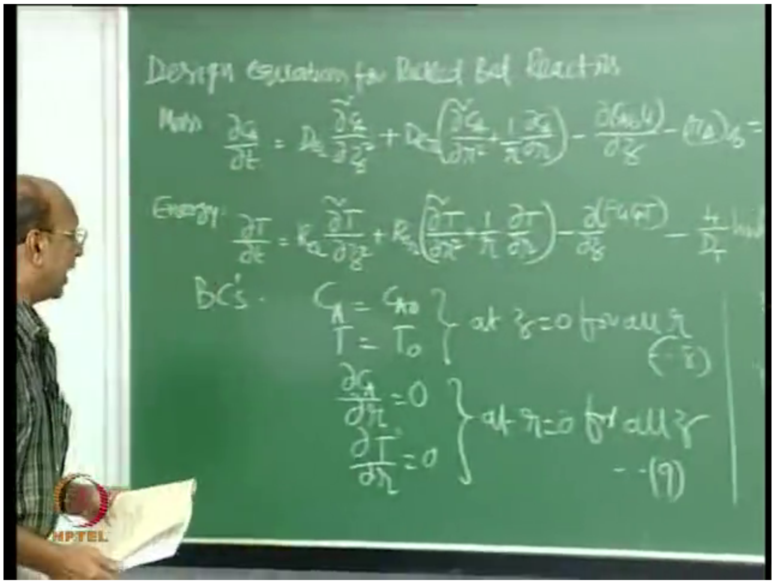

Okay anyway, so these two are the equations which we have derived in the last class, okay and you can see the meaning of this equation this is 6, this is 7, okay. So then you can see this meaning of course this is the accumulation term where we have you know normally we do not take that into account accumulation because all steady state reactions so if you do not have steady state reaction then you have to take this term then this is the axial dispersion term this is axial dispersion coefficient correspondingly that change in concentration with length and this is the radial dispersion term and radial dispersion term will have this because of the cylindrical coordinates, okay.

So then this is the actual convection term flow actual flow and this is the rate of reaction term, right? So in ideal plug flow what we do is we block this, block this, block this steady state and then you will have only these two convection and reaction, okay so that is why if you say flat velocity profile this u is same across any cross section but in fact it may not be true but still we are taking but the moment you imagine that we have some kind of axial mixing then and radial uniformity is not is assumed radial uniformity and the axial mixing it goes like this, okay.

So in that case this is blocked and only this is there of course if you take this also this term will not be there steady state if you take. So but most of the time in the last reactor theory class I have proved that most interesting thing will be only radial dispersion but not axial dispersion, why? Under what conditions I told that? Do you remember, again this is another quality of our all of us you know as students we remember only the current things not last semester what has happened previously what has happened I think what we remember is only alphabets which we studied in the schools, that is all afterwards nothing we do not remember at all none of you remember? RTD during RTD time we have done that if you have l by dp certain ratio you can safely neglect axial dispersion, okay do you remember those numbers? l by dp for 5 percent away from plug flow if you want to be 5 percent away and it is I think 54 or so, okay.

And if you have if you want to have only 1 percent deviation from plug flow then it is 5 times of that I think 190 or something it comes. So that means l by dp must be 190 that means if you take 1 centimeter particle the length should be minimum, so 1.9 meters so this criteria is easily followed in industry most of the time in industry the height of the packed bed will be 4 meters, 5 meters around 20 feet, okay and not 1 meter, 2 meters so that is the reason why and diameter if the particle will not increase more than half an inch either 10 mm or 12 mm.

So that is the reason many times you do not have to consider this term, okay but most of the time you have to consider this term again, why? Most of the time the moment you want to go to I mean best thing is to say that no I do not care about any non-ideality this is ideal world so though I will follow only ideal world so then I take only plug flow means fine, no problem nothing is there only these two steady state reaction, okay think I say think, think, think extend your memory a little bit of thinking, Prahuv, Prahuv I will ask I will come to you the question is clear or not clear at all, I know this is way that I say matrix movie you are here but literally you are not here you are somewhere else your mind somewhere else, okay.

What I said was most of the time we can neglect this you know why we can neglect this, all this smart question smart answers please leave I say, smart answers will be good for MBA, okay but not in engineering I tell you definitely not in engineering all the smartness I think you know management you can use but in engineering you should be solid you should know or do not know, okay in science also, right? Because I said so what is that I said so, I said so many things but are you following all those things? Okay there again you do not follow, okay but right now you will follow because you want to escape temporally the question, so that is why he said you said so that is why it is right as if you are believing me every second every minute I have just explained the length of the reactor if it is more than 190 packed bed reactor 190 means if size of the particle is 1 centimeter particle size, right?

So the minimum length for ignoring this term should be 1.9 meters so that means L by dp must be, let me write 190 L by dp, right? So if I have 1 centimeter particle the length minimum should be 1.9 meters this we can prove through (())(5:58) and distribution studies where we have discussed about axial dispersion model, okay there I proved that. So this condition of 1.9 meters and normally we do not use beyond half an inch particles, half an inch is 12 mm so 10 centimeter 10 millimeters also very frequently used in industry so that is not varying much but whereas the length of the reactor will be 3 meters, 4 meters, 5 meters, 6 meters, 20 feet also 20 feet is almost around 6 meters, right?

So that is the reason why axial dispersion will not affect us the conversion is not affected by axial dispersion most of the time in the industrial reactors, whereas next I asked the question this term this is the radial dispersion term that cannot be neglected most of the time can you think why, first of all why the term came radial dispersion term why it has come there first of all what is that we are assuming there, radial non-uniformity, okay good that is why the term is there now just imagine in the actual operation under what conditions we get radial non-uniformity or when the diameter is, comparable to size at the particle is, it will be uniform if it is small diameter it will be very uniform flow, okay if you put only in 1 inch diameter only you know maybe 1 centimeter particle flow will be uniform but only thing is (())(7:39) will not be uniform because somewhere you have more wides somewhere you have large wides and all that but at the whole in the cross section the flow will be uniform, right? But when you have large cross section and not that it is not only large cross section that is one factor most important fact is most of these reactions either exothermic or endothermic you have to either remove heat or add heat when you are removing heat it creates temperature difference from the center to wall because wall is the lowest temperature when you are removing or center maybe the highest temperature because you know reaction is taking place across the cross section and packed bed is a lousy conductor packed bed is a really lousy conductor because you have wide edge plus solids and fluid in between all kinds of things are there.

So that is why it is not a good conductor, if it is not a good conductor naturally you will have gradients, okay that is the main reason if it is endothermic reaction you supply heat from outside and wall will be at high temperature and center will be low temperatures and automatically whenever you have the temperature gradient immediately concentration gradient also comes into picture, it is called which effect? Soret effect in mass transfer, okay the other one is (())(9:01) effect or something is there which is reversed, okay.

So that is the reason why most of the time this term is very very important for us, you know logic is simple most of the time these are reactions either exothermic or endothermic either you have to remove heat or add heat. So when you are adding heat or removing heat definitely there will be concentration temperature gradients across the cross section this temperature gradient automatically creates concentration gradients.

So that is why this term and this term are much more important in normal packed beds when compared to these two axial dispersion terms, okay name the other thing is okay fine so this is the convection term this is rate term this is again convective heat transport term and this is the heat removal through the wall, okay and here you have again heat generation term, okay good. So these are the equations and these are the differential equation so I have to write definitely the boundary conditions some of these boundary conditions already you know this is Ca equal to Ca not, T equal to T not at z equal to 0 for all r and I also have dou Ca actually all these things are bulk please remember because it is pseudo homogeneous model, okay pseudo homogeneous model.

So pseudo homogeneous model means we are talking about a packed bed where we never fell for the packing that is present there we treat as if only fluid is only through the packed bed, so that is why it is bulk concentrations, right? Somewhere please write down otherwise you may be confusing all these temperature is also is bulk because I did not specify in the beginning the reason is that we are only talking about pseudo homogeneous models pseudo homogeneous means there is no presence of even through there is a presence of solid we do not feel that there is a solid, right? As if it is empty cross section where only bulk flow is taking place that is the reason.

So dou Ca dou r equal to 0 dou T by dou r also equal to 0 these are all at r equal to 0 for all z.

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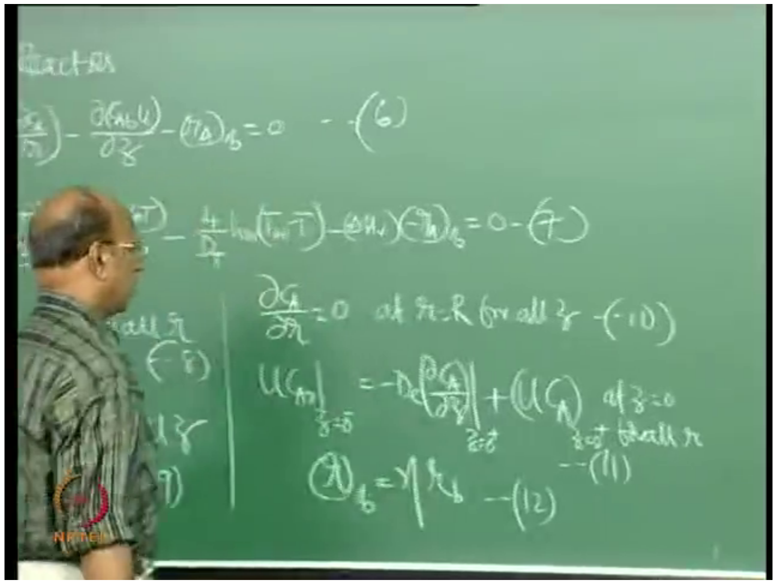

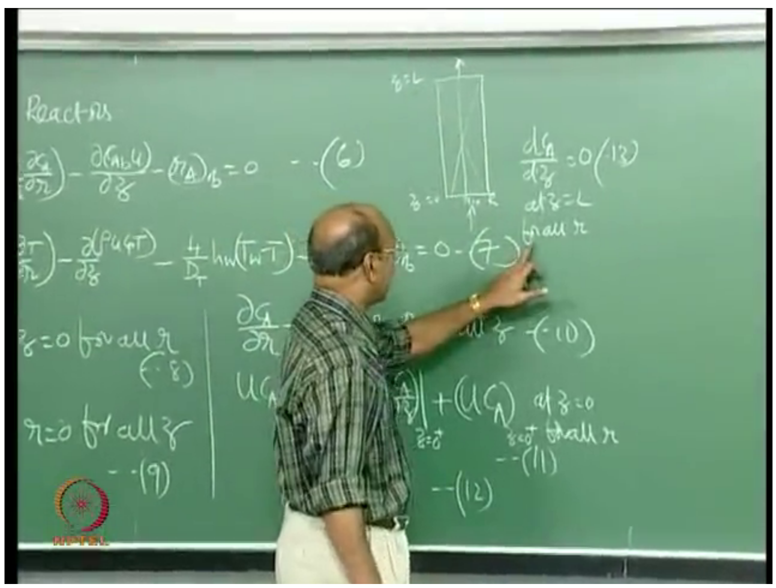

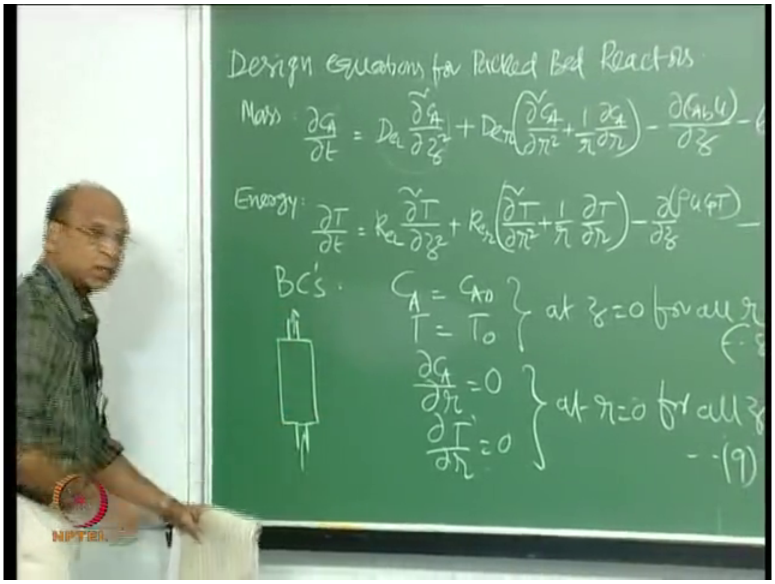


So another condition is I think I will write here dou Ca by dou r equal to 0 at r equal to capital R for all z I will ask the meaning of this, then we have another boundary condition Uca not minus D dou Ca by dou z at z0 plus uCa 0 plus this is another boundary condition at z equal to 0 (()) (12:38) for all r and we also have another without forgetting rb.

So if I give the numbers, what was the last number actually? 6 and 7 so this is 8, 9, 10, 11, 12, good. So again some physical meaning, Kaviya? Is this correct what is the meaning of this equation 8? Where are we talking about this boundary, z equal to 0, z equal to l now it will be very clear this is r, 0, capital R, okay this entire thing is packing things go inside they come out is very easy now no.

So z equal to 0 for all r what is the meaning of for all r? But it has to be specified clearly what will happen if I do not specify? So that means (())(14:15) when that is only at z equal to 0 the material is entering by plug flow at the entry level, okay so that is why along the radius there are no non-uniformities it is going as if the concentration velocity you know temperature everything is uniform across the cross section when it is entering, one siting is entering then you have this problems, okay so that is why we have to specify that if you are do not specify that then we will have a problem of what is the temperature here because these two equations will give you information at each and every point throughout the reactor at any r at any z temperature and concentration if you are able to really solve these two equations without dropping out any terms, okay you will get all the information about the packed bed but normally we do not do it because as engineers we would like to simplify and (())(15:18).

So that is the reason why we will only drop out some terms important terms and important terms through them away so that is the reason why we do it otherwise if you are able to do this as a pure mathematician you get all the information solution of this may take place I mean you may get only in 10 years but still you will get beautifully all the information, so that is why all these points are very important this one this condition, Swamy you are telling something what is this condition? (())(15:51) what is (())(15:55) symmetrical but where are we talking, at the center because of the symmetric diffusion the gradient equal to 0 beyond that there is no transport, okay so that is what either for temperature and concentration and this is at r equal to 0 for all z what is the meaning, at any point draw any line there along the z line so this is valid, what is this one dou Ca by dou r equal to 0 at r equal to capital very good no mass transfer through the wall and which is valid for all z at any point because there should not be any holes in the reactor, okay but this is what is the condition I was telling if it is a membrane reactor this condition will be different you will have some flux glowing through the wall, okay that is again diffusion flux (())(16:51) you can take that is the one which is going at r equal to capital R along all z some flux going out for membrane reactors the same equations exact we can use for membrane reactor also, okay good.

Then this one flux balance at the bottom so what is the meaning of this term, what is the meaning of this term, what is the meaning of this term? I think I will ask this people they people have been exposed last time, you remember Rachit, Karthik? What is the meaning of this at z equal to z minus at z equal to 0 minus just before entering here you have this equation and now you have this and this what is the meaning of that, because you know at just at the place of entering we are assuming that we have everything entering by plug flow flat velocity profile indirectly coming in the other boundary condition also, okay.

So after the moment it enters because we have axial dispersion term here then this will split into diffusive flux and convictive flux I told you no example if I put lot of perfume here and then stay in the room without like this no still air room there is no moment of air so then it will be only by diffusion which is this by concentration difference if someone puts me my behind any fan then you have the convection.

So the moment it comes into the reactor because of the dispersion in the reactor you have some by dispersion, some by conviction and what is the name of that boundary condition? Danckwerts boundary condition Danckwerts in fact intuitive boundary condition so excitingly I told you last semester that one because later this by intuitive boundary conditions later all the people try to prove him wrong and all the you know they could not prove him wrong he was right these are the best boundary conditions for a packed bed, right?

And of course the other boundary condition at the outlet was Dca by dz equal to at z equal to l, 0 that is also another one which is not required here but still I think I can write, where do I write? Okay there I think okay Dca by dz equal to 0 at z equal to L again for all r, okay that is another one this is 13 and equation 11 and 13 are called Danckwerts boundary conditions Danckwerts intuitive boundary conditions, okay you are not feeling well? Why I cannot say for all r all L no z equal to for all r why I cannot say, why you cannot say tell me the reason what is your doubt why do you feel that that is not true, discuss I say no problem whatever you have discuss if you ask Prabhuv, Prabhuv will give you very smart answer, Prabhuv what smart answer you have for that (())(20:52) by dz equal to 0 he says at z equal to L but since I cannot say for all r I will give you the clue I also told you sometime back you also should have definitely learnt that there are what are called open open vessels and closed closed vessels anytime remember, Renita? Abhinav long time I looked at you tell me.

What are closed closed vessels and open open vessels? Not boundary conditions I am just asking vessels how do you define a closed closed vessel in chemical reaction engineering, not English wise English wise closed closed means closed one closed is enough why two closed flow you know it is a reactor flow it has to enter it has to come out, so both sides you will have to have flow otherwise after sometime it will break with loud noise because once you have flow other is not coming out what will happen, okay pressure will increase so much then dom, open open is in flat velocity profile not there but what is the meaning of open open, where? In the entrance there is no mixing what you call that if there is no mixing what you call that, but what do you call that there is name nowhere is (())(22:51) mixing equal to 0 plug flow.

So definition of closed closed vessel is the material in any vessel if it if the material is entering by only plug flow leaving by only plug flow then it is called closed closed vessel, okay examples are packed bed in fact how packed beds normally designed is I am going to Lkg all the time I say, see this is one lousy we have designed in packed bed reactor but which is the closed closed vessel example because here I have small cross section here also small cross section when compare to this, right? So definitely velocity will be high we know that when we have very high velocity you are moving towards plug flow, right?

So this is the reason why we will say here that I have at all r because r is only here, okay at all r I have the plug flow that is why at all r Dca by dz equal to 0 at the outlet, okay and I gave the explanation again I do not want to give the explanation that takes I think minimum for me 15 minutes to explanation that why Danckwert said this is okay easily understandable even Danckwerts could explain this one very easily but in this place why Dca by dz must be equal to 0 he has beautifully physical intuition he has had and then he explained that in terms of Dca by dz equal to 0 is the correct boundary condition at the outlet you have to read that 1953 first paper on residence and distributions we also need some kind of history I say you should know who are your grandfathers in chemical engineering, okay.

Some of us are already grandfathers because we are about to retire, okay we may not be that great chemical engineers but still promotionally a grandfather but great grandfathers also you have to remember Danckwerts I think that is a beautiful explanation what he has given 1953 paper I am not I have that paper but I do not want to send to you because if I send it to you it will be e-pollution unnecessarily because I know I will send it to you it will be on the computer you will never download you will never read, why unnecessarily wasting computer space so that is why otherwise you know there is interest I could have sent many many papers I have some wonderful papers one or two Danckwerts paper not Danckwerts (())(25:21) papers wonderful papers where without maximum mathematics with minimum how beautifully he has told yesterday I gave that condition no dynamic program condition where 0 to you know in and out dou of dou dou by dou r of 1 by minus ra into dxa equal to 0 intuitively he told that that must be the condition for optimal design of any reactor I mean the plug flow reactor or packed bed reactor later people proved that dynamic programming through dynamic programming you get the same condition that is what is the great intuition for engineers that is required scientist can have time to do things and then finally you will say that yes his intuition and also mathematics both are matched but engineers without mathematics also they should have intuition which later can be proved by mathematics.

And if you have that kind of intuition then you have you are excellent engineer, okay because every time if you start proving you will not have time to do things no as engineer, engineer has to run the world, okay I told you no, I have my famous thing engineers around the world, doctors save the world and who are the people like Brahma, Vishnu, Maheshwar? You know we have three gods you know very famous gods, Brahma, Vishnu, Maheshwar, so what is the job of Brahma? (())(26:53) what is the job of Vishnu? Protect, what is the job of Vishnu I mean Maheshwar? Destroy.

So like that we also have this you know as engineers we run the world we produce things also and then run the world. So Brahma and Vishnu in one place engineer, okay I really said of of 50 percent 50 percent otherwise you choose you know if you are theoretical engineer not producing anything you are only half of the body of those two and anyway there are so many things which I can tell you but I think I thought I will complete packed beds today I am not able even start packed beds today, okay anyway.

So all these equations this is the reason why you know we can say that if I have this kind of flow, right? So then I can say that I have at all r the dispersion is 0 flat velocity profile then I can say that condition is right that is only valid for closed closed condition, okay then we can have the open open where the materials enters by dispersion and also leaves by dispersion, so that is an example of tubular reactor normal tubular reactor where we have this is the tubular reactor there is no small tube here and under small tube there for things to come out, good.

So this is the tubular reactor where material enters by that means same dispersion whatever is happening inside here if I have the dispersion same thing also is happening here same thing is also happening here. So this is called open open vessel and this is called closed closed vessel, okay good I think this class has become a joke class and I want to finish this packed beds and then start fluidized beds, okay good.

So now we have the terms normally what we have to use, okay this equation 6 and 7 we can choose that means if axial dispersion is not important this may not be there, this may not be there and if radial dispersion is important this will be there and this also will be there because both are connected, okay but under one condition both are not connected this you may have radial dispersion and you may not have, okay for adiabatic reactor I think I instead of asking you that answer for adiabatic reactor what will happen, which terms are important in this? Adiabatic reactor means there is no heat input no that means you are not taking anything from the walls, Prabhu? For adiabatic reactor which terms are important equation 6 and 7, important or not important that is not there adiabatic means totally this is not there, okay.

So out of the rest of the terms also some will not be useful some will be useful because there are so many conditions here in this I mean with those two equations you can imagine for example if it is adiabatic reactor and let us say adiabatic very small diameter, what are the terms which are important? I think this you should be able to think I say, adiabatic system but diameter is small, this one that means axial dispersion term is there, radial dispersion will not be there, why? Because diameter is small you can expect uniform things, okay.

So then this one will not be there? This has to be there this is the main convection, okay then this is the term, okay but now Reynolds number is more than 40,000 in that reactor this also will not be there study state this also will not be there, okay. So depending on each condition either flow condition or the heat transfer condition whether you are heat removing you adding or adiabatic . So depending on that you have to choose the corresponding terms, okay.

So like that we have to simplify them and I think I have to give the conservative equations where normally people use, okay. So tomorrow I will give I have a table which I have taken from H.H. Lee there is a book heterogeneous chemical reactor design heterogeneous reactor design H. H. Lee, okay good book, so that is why I know my notes always will be from various books but I am mentioning Carberry I will take something and Froment and Bischoff I take something, Lee I take something this information is good for us but I think what is the uses I am disappointed most of the times because after the examination is over or even before the examination is over if you know that this is not coming in the examination you never bother to remember, Prabhu sad no?

What is the ultimate idea I say? Ultimate idea is when you are a chemical engineer there are something which you should know, okay at the end of chemical engineering but now I think you do not know chemical engineering spelling also you will forget very quickly I do not know chemical engineering spelling how may people write, because most of the time we write chem engg no? That is all I think everyone things that that is the expansion of chemical engineering that is why it is very very sad otherwise there are so many nice things, okay and I was also telling in the department you know like see B. Tech now I think B. Techs have you know it will come to M. Tech also it is not very far B. Techs you have a choice no not to do the project and go for only courses, I discussed in the department I think in chemical engineering we are so lucky we have so many flow charts, so many problems and if you give that problem as a project student will learn so many things in that, see one project can be solving these two equations I say where I get fluid mechanics here velocities and I get heat transfer there, I get reactions there, I get transport phenomena there because dispersion and all that, that is correct I know that is traditional way of doing chemical engineering project throughout the world but I think in IIT last 25, 30 years I have been fighting this.

So give them that kind of projects where they learn everything but no, no these people are very very intelligent so we should not give them that project, we have to give the research project, research project anyway they cannot do so finally what is the solution so no project. So really that is why so many things they will learn if they solve the this kind of equations in there project same thing after 5 years I tell you M. Tech students are not interested in the project that is the logic why B. Tech students synet also expected unfortunately synet also thought that when they are not interested why should be give them project let them take courses.

So that is why you also do not do the project no, M. techs, okay. So after 5 years everyone will realize that M. techs are also not doing then course work another four courses you do not learn anything anyway, so that is the kind of thing what is happening so many interesting things are here, okay maybe I think will tomorrow I will write I think you can now run.