Chemical Reaction Engineering 2 (Heterogeneous Reactors)
By Professor K. Krishnaiah
Department of Chemical Engineering
Indian Institute of Technology, Madras
Module 01
Lecture 34
Conservative Equations for Packed bed Reactor design

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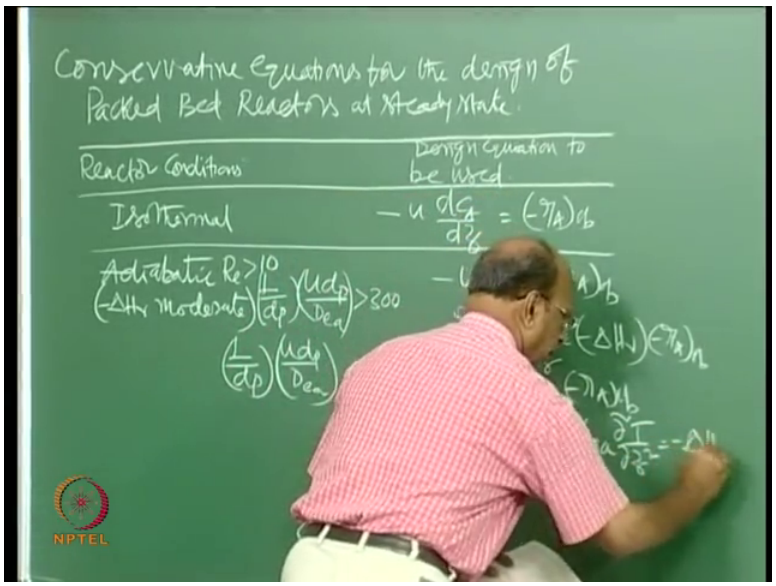

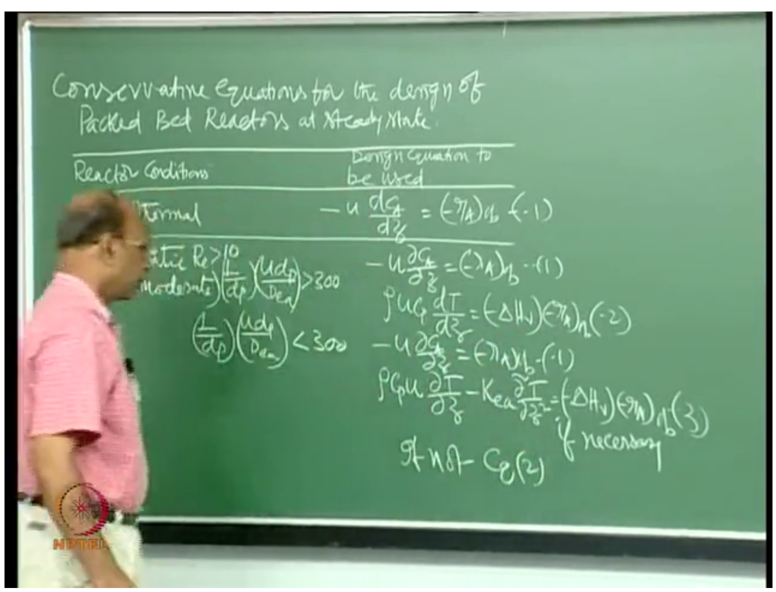

Conservative equations for the design of packed bed reactors, this is the one I think will it be sufficient here, okay I will try this is reactor conditions reactor conditions, then this is design equation to be used, good. So first reactor conditions if it is isothermal, okay see we are referring to the same equations what you have written now you have dispersion term, you have dispersion axial, dispersion radial so then you have convictive term, right? Then you have unsteady state term and reaction term, okay this five and conservation equations for the design of reactors at steady state so straight away dou Ca by dt will go, right?

Now you have isothermal that means you have completely energy balance equation out now you have only mass balance equation dou Ca by dou T out and it is isothermal, okay so most of the time we are neglecting not radial axial L by dp is very large, okay most of the time industrial latest, that comes later so radial I mean axial we anyway neglect because most of the time L by dp will be greater than that 150, 130 like that, so then only one term now radial dispersion term is there because there is no heat transfer, no isothermal and all that so you can also assume that we have only radial uniformity so finally you will have this equation if I simplify that you will get minus u dCa by dz equal to that is the equation to be used this is just nothing but I was telling to you know W by Fa not depending on the units of minus ra kg per catalyst means W by Fa this you can convert this as W by Fa not equal to integral 0 to Xa dXa by minus ra you can convert that.

So for isothermal case these are the conservative equations we do not have to worry about all other term most of the time when you have isothermal we can use only this is the convictive term and that is the rate of reaction, okay all other terms you can neglect there. So now if you have adiabatic case this is 1 when you have adiabatic case adiabatic case means straight away the other term will go that 4 by dt or u a delta ua da that delta t, okay so that will not be there so then we have different conditions in adiabatic case if I have adiabatic case means first of all adiabatic case when do you use isothermal is delta Hr approximately 0 adiabatic means you normally use adiabatic reactions when you have the delta Hr somewhat intermediate maybe around 20 to 30 kilo calories per mole, okay so approximate values they are not universal values that everyone must follow that, okay how serious temperature again anyway you have to simulate and then try to find out but definitely you cannot go to adiabatic if you have heat of reaction around 60, 70 kilo calories per 60, 70 is very high for example above an reaction and all that.

So that is why you have to go for only (())(5:08) so then you have to only go for non-isothermal non-adiabatic that means heat must be removed, okay. So these are the general thumb rules. So that is why when I write adiabatic here you can also write delta Hr moderate and we have feeling that around it maybe 20 to 30 kilo calories per mole, okay so under those conditions if you have this still reactor conditions, okay if I have L by dp this is one group udp by Dea if it is greater than 300 you got the meaning of this what is udp by Dea? What is udp by Dea? What is the number of is there any name for that? That group (())(6:11) you told something? It is peclet number but pecklet number based on particle diameter what is that we are now multiplying by, what is this called L by dp called? Aspect ratio, okay.

So when you multiply aspect ratio with pecklet number based on particle diameter you know what you get cancel out dp dp, then also it is a pecklet number but based on reactor length. So pecklet numbers sometimes they are expressed as length of the reactor answer sometimes particle diameter. So if this column pecklet number, okay or reactor pecklet number if it is greater than 300 then you have to use because it is adiabatic so definitely energy balance also will come, okay temperature also dou Ca by dou z equals to minus raob and other equation is dou Cp dt dz equal to minus delta Hr minus raob in fact this is what we have already done when we were drawing those graphs and all that, okay.

This one if is solve I will get T as a function of Xa T as a function of Xa maybe you know these symbols are different but finally you will get the same thing Fa not and all that, Savita is blank totally blank this equation is nothing but your mass balance energy balance equation for adiabatic system what we have down last semester and also sometime back also I have shown you that, okay.

So that is why this is very simple to solve because this is now only ideal plug flow that means again we are neglecting radial because when you are not removing heat so there is no temperature gradients across the radius, okay only temperature gradients in the axial direction that is what is this dT by dz so I mean spend some time you know to understand the physics of the equation that is why I am trying to explain you could not write because that physics still has not gone into your blood, okay.

And in chemical engineering similar equations will come in almost all subjects, okay and I do not know whether you noticed it or not maximum order of differential equation what we used in chemical engineering is second order beyond that you do not go, okay only civil engineering people will go mechanical also is same, aeronautic people also same all most of the engineering problems the second order differential equations enough except civil engineers where they use for bending what is that beams and all that, okay cantilever beams.

So they only go to the four of four and to the four of five all other second order differential equations so that means only two boundary conditions we require for every system and all that, okay. So that is why this is again already you are familiar with and why we are neglecting all other terms like radial dispersion because you are not removing heat temperature is uniform that will not create any concentration gradient that soret effect if you have concentration temperature change along the radius then that will create automatically concentration difference.

So that is why we have to take radial dispersion term but here it is adiabatic we do not have to take, good? So then if it is less than this this number if we have L dp into udp by Dea axial dispersion number less than 300 then it is only necessary you have to check and, sorry I think I have to also write here another condition this condition plus Reynolds number condition Reynolds number greater than I think here I can write this is common to both Reynolds number greater than 10 if you have again Reynolds number greater than 10 and this condition less you have the same equation dou Ca by dou z equal to minus raob and you can use dou Cp dou T by dou z minus Kea dou square T by dou z square that is the axial heat transfer term maybe necessary it means minus raob if necessary, okay.

So if I give number this is 1 this is again of course 1 this is 2 this is again 1 this is 3 if necessary if not then you have same thing equation 2 necessary means you have to see you have to take this term and then solve the equations axial term temperature term, okay and if your conversion is almost same even if you take this or do not take this then this is enough equation 2 this is enough, okay.

So with computers and all that now one has to do these simulations, good? So that is why this is only just caution whether it is really required or not one has to check depending on the problem, good.

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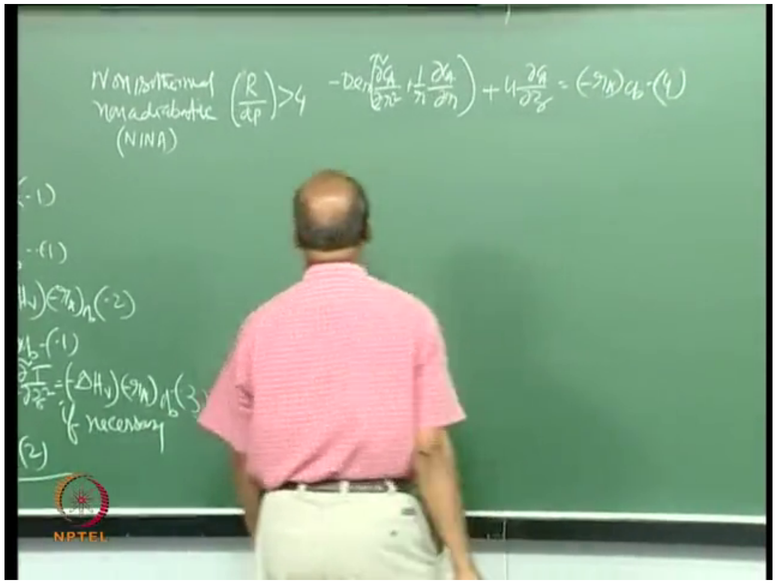

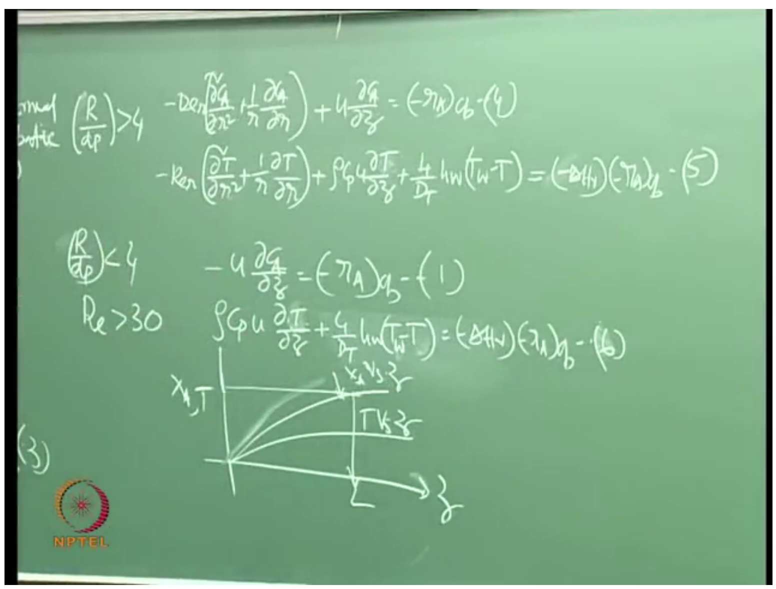

So that is the one then you have non-isothermal non-adiabatic case same similar table this is end of this, so here we have non-isothermal that is the reactor conditions non-isothermal non-adiabatic, so sometimes we call this NINA reactor non-isothermal non-adiabatic, right? Some books will give NINA.

So under these conditions if I have R by dp greater than 4 then you have to use this equation, okay that is under this it will come this is radial dispersion dou square Ca by dou r square plus 1 by r dou C by dou r I think I will extend beyond this boundary u dou Ca by dou z equal to minus so this is equation number 3, this is equation number 4 and this we have to also use ker dou square dou square 1 by r dou T by dou r plus dou z plus I have 4 by Dt this term also will come hw Tw minus T equal to minus delta Hr minus raob, so this is equation number 5, thank you thank you still alive and kicking, okay.

So dou T bu dou z so that means this is the only serious case why you know r by dp what is the meaning of r by dp? Radius by dp so hoe many particles you can put across, up to 8 across the cross section, okay. So if you are putting more than that heat transfer effects will come because I told you packed bed is a lousy conductor, okay so that is the reason why you have to take those things but you see here axial dispersion neglecting, correct no? Axial dispersion neglected at in fact axial heat conduction can always be neglected axial one except here it is only necessary just to know if you do not see much difference this also you do not have to take Kea is a axial heat dispersion term, okay that heat conduction term, okay good.

And I hope you know what is e and what is de this e and this e effective diffusivity where we are clubbing all the mechanisms like for example effective diffusivity is a combination of configurational diffusion, bulk diffusion, (())(16:58) diffusion all there diffusions together we do not know how to separate them mathematically we know each expression we can if you know we can find out otherwise it is effected parameter where through experiments Dea is evaluated through experiments and then fit in terms of correlations, right? In terms of velocities in terms of both particular sizes and all that, good.

So this is the another expression and now if I have row R by next one dp less than 4, so R by dp if is less than 4 which are the terms that may go out there? You got cr he is blocking you, what are the terms you have to take what are the terms you have to neglect? Use some physics use some brain you know I think totally do not close I say, why? In both the places? That means mass balance and heat balance in both the equations, both but then why not mass if heat is neglected automatically you may not have concentration gradients no but what is the meaning of Rep R by dp less than 4, smaller diameter of the column.

So radial uniformities can be expected so both will disappear, okay that is the logic you know that is the reason why I gave this test I thought you know you will use that kind of logic and then quickly finish it off, okay but where is the logic every logic is only in the examination hall afterwards it will not work nothing will work, oh my god every time it is boring I say every time you have to talk about only exam, exam, exam, okay.

That way I like this our doms department you know there management the guys who do management they have passion for doing management in fact I told the recess even thesis scholars are so passionate then I told them why don't you come to engineering departments and then walk across everyday some two hours around that so that your some of your passion will diffuse from you and then go to this department because there is 0 diffusion gradient is there so that is why easily it can diffuse.

So chemical engineering department 2 hours, mechanical engineering department another 2 hours, okay like building wise really they have tremendous passion engineering absolutely no passion only examination, okay so that is why I think you know always they sit in coffee day and also discuss management students, there system is quarterly system what you are studying in four months they are studying in two months all (())(20:25) credit courses, okay.

So that is why they have passion otherwise they cannot survive in management because it is usually so boring subject no, and what is management? Common sense and logic, okay that is all but I think most of us will not use common sense most of us do not use logic in engineering. So that is why we do not have that passion but they try to use and you are not answering (())(20:53) are there getting lot of salary we are not getting that much salary you have to depend yourself I say I have to put the question I have to answer also, okay because there starting salary maybe 20 lakhs and your starting salary is 20 thousand, okay so that is why you do not have passion and they have passion this is what I have thought once with one big company man and then afterwards he never looked at me and then I was member and I was removed, okay.

So why I the I just asked why I think you know in IT industry people should be paid more, what is that they are doing extra when compared to an engineer, okay because engineer is doing his duty in the plant he is doing in IT person is doing whatever project is given in the IT industry, okay why they should be given lakhs and lakhs and where these people are given only thousands, there was no answer except anger, okay that is no answer if that answer and anger should have been better but anyway, good so this is also we have another condition here Reynolds number, Reynolds number also is based on particle diameter any packed bed I think all the time we only base the based on the particle diameter, okay so that I do not have to repeat again.

So in this case we have equation dou Ca by dou z equal to minus raob and row Cpu dou T by dou z equal to minus delta Hr and minus raob, so this is again equation 1 other equation is equation 2. See you have to re-appreciate that engineering mind you know simplifications even though I have non-isothermal non-adiabatic and you know fairly large amount of delta Hr and all that still I use only these two terms, sorry you have heat transport term that will come no that one is plus 4 by Dt hw T minus Tw it depends on, okay depends on your adding or you know endothermic or exothermic term, okay.

So this is equal to minus delta Hr minus raob then this equation will be not 3, 5, 6 so these are the equations that is all what we have to use, okay please remember them I think you know even though you are not in chemical engineering sometimes I think it is better to know this, okay. So I think there are so many beautiful things are in chemical engineering because there are so many people are (())(24:14) upon then anyway I do not want to do anything because sometimes it happen if you have too much work you do not do any work because you do not know where to start, okay.

So maybe because of there are too many concepts and too many beautiful things here people to many things are there what do I do so leave it maybe that is the reason why you are not interested otherwise you know in other countries USA, Germany and all that chemical engineering is in fact chemical engineers who are getting the maximum salary in US when we were studying I think that went on till maybe 80-85 but of course no one can beat them in medical doctors in the US I think they get maximum, the next one out of all engineers who are chemical engineers I am talking about 70's and 80's, okay after IT came and all things have gone down only they came up too much (())(25:05) so came out, okay.

So that is why so many beautiful things are there I think you know think you see you are taken so many courses you know at least in one course have you solved this equations, at least in one course and even you are supposed to solve this in transport phenomena because transport phenomena here you do not have time to solve here is in reaction engineering course my idea is only to give you the concepts not the mathematical techniques mathematical techniques you are learning from mathematic courses plus transport phenomena, transport phenomena is 30 to 40 percent concepts the remaining 60 to 70 percent solving solutions there you have to solve, okay then you will know then you will really enjoy if you solve those equations then you how to plot you know in all these things what you get at the end you always get temperature conversion and length of the reactor that is all what you get because Tx and you have what is other one, Ca.

So what you have to generate here is the graphs this is Xa and T, okay Xa will increase like this this is Xa versus this is z Xa versus z and the other one is temperature, so depending on whether you know adiabatic and non-adiabatic cases and all that adiabatic means simply this also will be another line like this, right? So now adiabatic case means depending on heat removal or heat addition you may get like this this is T versus z these are the things what you do.

So you are getting here if someone asks you okay what is my reactor length for 90 percent conversion so then you know you go to 90 percent here that is the reactor length where you will get even the outlet temperature, so that is why here you cannot have the unilateral solution you have to go by most of the time the technique used is finite difference method you take small delta X and then calculate small delta z and also temperature changed there like we had so you have no I think the second order differential term how you have to expand I terms of finite differences I think definitely someone would have taught you in numerical technique courses and all that, okay so those are the technique what we use and try to solve them convert them into algebraic equations and then try to find out, okay.

I do not have time to do that I mean if I have only packed bed reactors alone then we could have tried this I have to do so many things because in this course idea is only to give the concepts, okay and of course to make you comfortable I leave it off you know some problems so that you are also do not feel that you have done only concepts and then no actual solving the problems that the reason why we give assignments and all that, okay.

So that is why is surprising to me I also never solve all those things together when we were studying every time this going on like that that is why I was telling that at least give that in B. tech or in M. tech project M. tech project also is not that simply to solve all these equation then and design the packed bed if you are able to take all the parameters how to design the packed bed and also use these mathematics to get the solution then I think you know your confidence level will shoot up and if you are able to solve this any problem you can solve because you do not go beyond this order of differential equation so many boundary conditions, heat transfer coming, mass transfer coming and fluid flow coming, reaction kinetics coming, diffusion coming you know even the particle thing and all that, okay.

This raob is nothing but eta into rb, okay so all those things everything will come in reaction engineering so that is why at least even if you do not solve you remember that you have not solved anything, okay that is also very important and first of all you should know what you do not know, okay so then that is the first point first starting point for any learning I think (()) (29:37) there is a quotation you know the stepping stone for knowledge is ignorance but you should know you are ignorant that is most important otherwise if you sit here and then like this if you do I think as if you know everything you cannot learn anything because you think that you know everything, okay so that is why (())(29:58) that quotation is beautiful, okay the first step to learning is ignorance which you know that you are ignorant, right? Not I should know only you should know that you are ignorant no point in me for me knowing that you are ignorant I know that already, okay.

So no point in knowing again further and you also will know that I am ignorant, okay so that is also true it is not only it is reversible reaction it is not only one way, okay good. So tomorrow I will start fluidized beds and just to make you comfortable with units I will solve 1 simple problem because in heterogeneous systems units will make lots of mistakes indirectly I am also trying to couch you for examination so that you will not make any examination mistakes, okay that one simple problem I will solve how to find out a weight of the catalyst or conversion if the catalyst weight is given so afterwards I think we can.