Chemical Reaction Engineering 2 (Heterogeneous Reactors)
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Lecture 26
Isothermal intraphase effectiveness factor part 2

Ya we have been discussing about this intraphase effectiveness factors, last time we have derived equations for sphere, cylinder and also the slab cylinder we have done I mean sphere we have done and then cylinder and flat plate I have given the equations.

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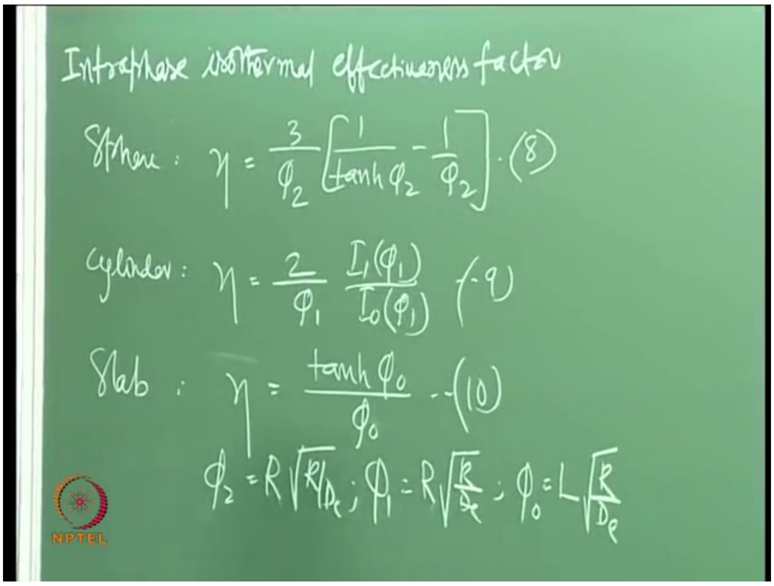

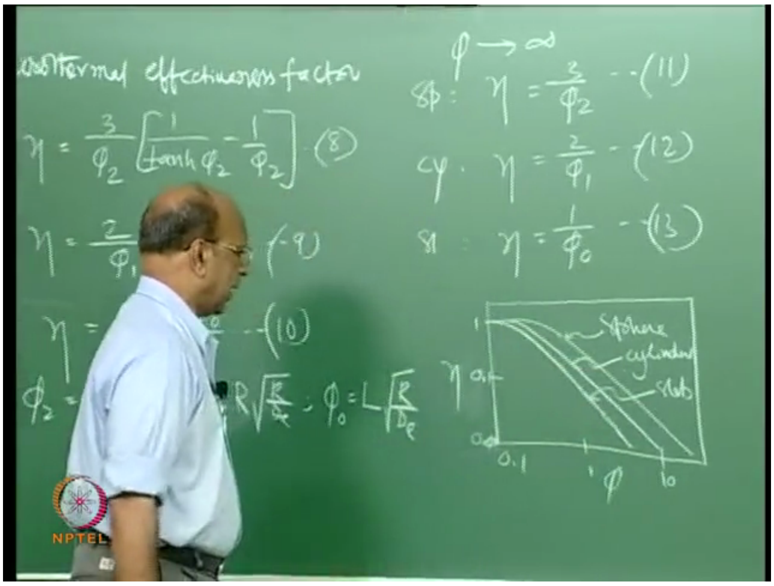

Now those equations were something like this intraphase isothermal effectiveness factor ya. So for sphere the equation we had was Eta equal to 3 by Phi 2 1 by tan h Phi 2 that is the equation and for cylinder Eta equal to 2 by Phi 1 I 1 of Phi 1 I 0 of Phi 1 this is the equation and for slab (())(1:40) Eta equal to tan h Phi not by Phi not ya so these are the these were the equations and what was the number here which one is 8 this is 8, 8, 9, 10, okay good.

So you now Phi how it was defined there as for example Phi 2 is defined as R by 3 that is what no just check Phi 2 Phi 2 Phi how the Phi is defined R into ya okay ya R into that is the radius of the particle and Phi 1 is also defined as R into square root of k by De because it is first order all for first order only you have derived that there the R is diameter of the cylinder in the second case, okay diameter of the cylinder I think why unnecessarily instead of asking you I better write there this is R square root of k by De Phi 1 is R square root of k by De Phi not equal to L into square root of k by De only thing you have to remember is R is the diameter of the particle, this is sorry radius of the particle, this is radius of the cylinder and this is half of the thickness of flat plates half of the thickness of flat plate.

So the total thickness is 2L so we are taking only L as the thickness, okay if you derive actually then you will know how you get only L there good okay.

So if I there is another thing here when I have large Phi Phi greater than Phi greater than Phi what will be tan h value, if Phi is Phi one more Phi take here this Phi is Phi one more or Phi what will be the value of tan h? Tends to 1 okay it goes to 1 for large value whenever we have Phi tending to large values you will have Eta sphere equal to 3 by Phi 2, for cylinder this will be 2 by Phi 1 and for slab this will be 1 by Phi not, so this will be 11, 12, 13 good.

So if I plot this Eta versus Phi so here maximum you will have only how much is the maximum by the way 1, 0.01, 0.1, 0.1, okay 0.1, 1 why 1? Isothermal ya because it is isothermal ya this is the one, this side we can have 0.1, 1, 10 that is the Phi value so you will get something like this ya so where this is for sphere, cylinder, slab ya good. So again meaning is very simple so at high Phi values I told you know usually greater than Phi that goes to slowly asymptote so then you will get actually this is the equation straight line what you have plotted there Eta, okay.

So for sphere and cylinder and slab that is the equation and problem is you know for this you have all three different curves for three different geometries this was observed by Aris, Aris is a cat so I think he was very smart, he observed that and then he thought that he has to made somehow all this, he wants to get only one one curve for all these three geometries, okay even though we use most of the times spheres and cylinders, slabs normally we never use it is only for academic discussion, right.

So the slab will have dimension you know the differential equation 0 that is why we have given here 0, this will be 1 and this will be 2, I will also give you some hand-outs so that you will know what is the differential equation for this, for this, for this, what to integrate, okay what are the boundary conditions all that I will just give you so that you can derive on your own.

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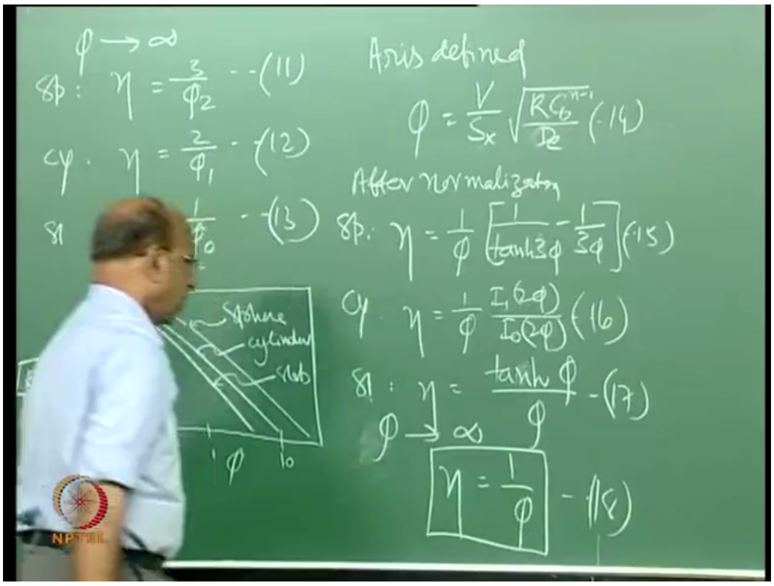

So once we understand that the next thing is as Aris said let us Aris defined very simple idea as Phi as V by external surface into square root of k C b to the power of n minus 1 by De ya with this can you tell me what will be the Phi value for sphere R by 3 not 1 by 3 ya R by 3, for cylinder it will be R by 2 and for slab it will be L again, okay.

So if you do that you will get a different kinds of equations like you know taking this definition originally in the into the derivation then what you get is after normalization this is a kind of normalization after normalization you will have for sphere Eta equal to 1 by Phi 1 by tan h tan h 3 Phi that is the equation.

For cylinder Eta equal to 1 by Phi this is the equation I think I have to write the number somewhere, this is 13, 14, 15, 16 and for slab Eta will be tan h Phi by Phi, okay. So here for all geometries if Eta not Eta if Phi is going to large value only one equation you will have that is simply Eta equal to 1 by Phi, okay ya this is the value.

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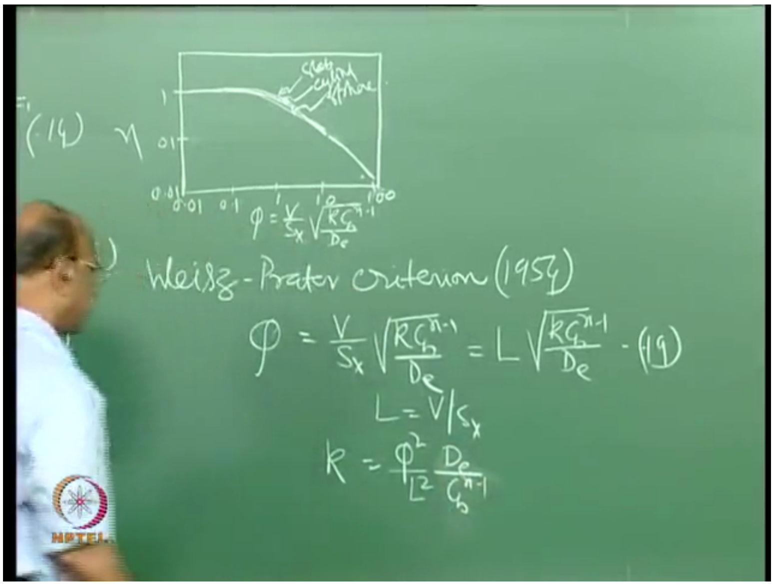

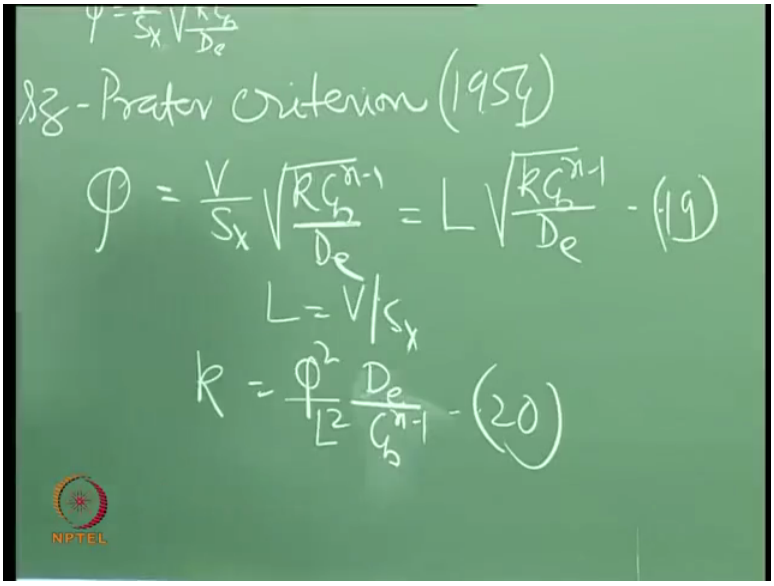

Now if you plot this then you will have external surface square root of k C b to the power of n minus 1 by De this is Thiele modulus, this is Eta, again 0.01, 0.1, 1 this side you may have 0.01, (0.1, 1, 10, okay) this is 0.1, 1, 10 till 100. So then you will have an equation I mean graph like this not so much ya somewhere here only you will have a small difference this will be slab, cylinder, sphere but you get only one line here for all three and here also you will get only one line good right all three.

So now any geometry if I know Phi I can just go here if it is 10 I can read, or it is 0.1 I can read, if it is 1 there is slight difference that difference also maximum he says I think may be 15 percent or something to 18 percent also so but almost practically you can take that curve as single line, okay ya what (())(13:04) thinking very seriously ya that is all I think it is very nicely done at that time 1967 or so.

So now I will give you these things just for (send give to them) in the previous one ya (()) (13:34) is top most why very simple no for the same three, for same Phi that is 3, this is 2, this is 1 so naturally it will be less. So there it is interchanged because of the equations if you plot them that is why you know computer you can use and excel is very easy to plot just go and give that equation and you nicely see what is happening, okay if I able to plot ya.

So this side also there are some old ones, new ones but I need one, okay good. So actually we have taken here I have drawn this long time back you know four shapes even single pore also is very nice one for understanding the effect of mass transfer, okay and the effectiveness factor single pore, flat plate and cylinder and sphere. So through mass balance there is a differential equation with boundary conditions, next one is what is the concentration gradient equation next column, then you have effectiveness factors and how the Thiele modulus is defined, okay good Narsimha Reddy anything?

Lambda is you know Levenspiel uses you know lambda also is given in the last column, there is no meaning for that because this is the geometric factor is the R by 3 or R okay so that one is L, characteristic length multiplied by the other parameters like reaction rate and then diffusivity that is all, okay. So Levenspiel gives that in a slightly different thing in fact his notation and all that slightly different, he has also done something good there in that in Levenspiel book but this one I have taken mainly from Carberry, Smith and various books, okay not only one book, good. I think Levenspiel never mentions about cylinders so slab also I do not know but pore and sphere I think he mentions pore and sphere, okay good.

So this is the one and ya theoretically I can ask you any derivation in this again I have to black mail you with the examination that is only thing to get something out of you so that is the one. Carefully observed is there I mean really can use this graph for finding out effectiveness factor? See our idea is why we are doing all this is to find out finally what is the effectiveness factor for your catalyst if you are designing a catalyst, if you are making a catalyst and it is better definitely to have it is like examination you know so after the course is over you give the examination to test how much efficient you are in learning, same thing here after designing the catalyst pellet we put that into test and then see what is the real effect of you know the efficiency of this particular particle, right.

So for that we have to do this, if I know this Phi value for any catalyst I can calculate from this graph or I can just read form this graph or use anyone of these equations and calculate effectiveness factor but will this graph will be really useful? See yes, yes or no? Swami says no, why do you say no? You have to tell no reason when you say like this, when you say like this you have to do plus or minus, irrespective to ya ya it is irrespective of shape I will give you spherical particle only one shape, I am not asking between three shapes what is the efficiency, I told you that we have one particle where you find out the I mean you design the particle and after designing the particle you would like to test whether it is efficient or not what is effectiveness factor for this because that determines the kinetics, no Sidharth ya why it will be useful, what is the procedure to get effectiveness factor?

Student is answering: (())(18:02) either the surface area or probably the concept they can alter this one.

You have the particle there is no question of surface area variation and all that, you have designed already a particle with some surface area, right. So particle is with you, so after designing this particle you would like to find out what will be the efficiency?

Student is answering: Situation can be varied in such a way that the desired effectiveness.

So what do we get, I would like to find out a witness factor I am asking what is the procedure, you should know Phi ya okay ya if you want to know Phi what are the variables you should know ya (())(18:45) what are the things measurable, what are the things not measurable there? C b is measurable, only C b, surface area is fine but surface area is okay this is you do not need surface area you know this will be simply R by 3, R by 2, or L because you do not have to measure anything there, right and that too that surface area is only external surface area, it is not internal that is why S x external, okay and that is the volume of the particle, good.

Ya like exactly the same problem what you had with external effectiveness factors, here also you have problem how to find out k without any mass transfer effect without any mass transfer effect. So that is why there we went back saying that okay now let me define some other observable where I can measure everything, here diffusivities we have some correlations that is no problem at all, okay ya I will give you some some kind of correlations there later.

So you have some correlations so De may be possible for us to have some value and C b measurable these things I know R by 3, or R by 2 or whatever and then you have the k value which is not easy to get without the presence of mass transfer, particularly for heterogeneous systems, okay. So that is why how to avoid that, if you avoid that can you do something else, okay.

For this there are again many people have done but there are two people who did this Weisz-Prator Criterion Weisz-Prator you heard of that ya what did they do, Eta ya Eta Phi square not Eta Phi, simply eliminated the k value, okay this is very nice but later I think with experiments and all that they have also ya these people have done this criteria in 1954, okay good.

What they did was I mean they have not done exactly the way I am doing because here we have simplified, we have the definition of Phi as this is the one V by S x square root of k C b n minus 1 De which also can be written as some characteristic length L into okay where L equal to V by S x external, okay. So now simply take out this k and this is 18, this is 19, okay ya so k can be written as Phi square by L square into De correct ya ya ya right right right De by C b to the power of n minus 1 so this is equation 20.

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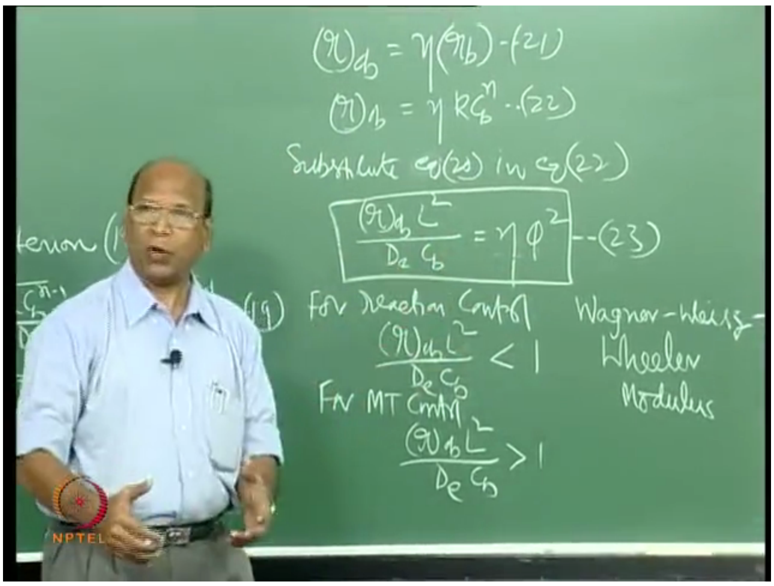

So now we go to our original definition of Eta not Eta r Ob equal to Eta r b right okay so here we have Eta if I have nth order reaction this will be k C b to the power of n minus 1 (not n minus 1) n, okay ya r Ob equal to, now we will substitute this this is equation 21, this you already know, this also you know for nth order reaction 22. Now substitute 20 in 22 substitute 22 substitute 20 equation 20 in equation 22 and arrange rearrange what do you get.

You get as r Ob L square De C b equal to Eta Phi square so this is 23 this is equation based for this Weisz-Prator Criterion.

So now they started telling that okay this is observable left side is observable, okay good. So if I have mass transfer limitations that means reaction is not controlling mass transfer is controlling or first let us state this curve here what is controlling till almost some point there ya here what is controlling and beyond this what is controlling? The first one is reaction control okay so here reaction control and other place you have MT control, okay good.

So under reaction control what will be the value of Phi and what will be the value of Eta? So r Ob L square De C b ya Eta is almost 1 and Phi is less than 1 so Phi square is still less than 1. So that is why you can have this criteria as if I have this modulus as less than 1 then I can say that I have okay mass transfer is not limiting only reaction is limiting so all these things are measurable.

So what you do is you after designing the reactor after designing the pellet what you have to do is you do the experiment, find out r observed you know the diameter so L you know and De effectiveness factor and also C b measurable sorry De is the diffusivity and C b is measurable. So if you put all that if it is less than 1 you can be very happy that the entire surface area can be used for the reaction.

In the other case for MT control naturally it should be greater than 1, why? Because Eta is ya Eta is 1 by Phi very good ya Eta is 1 by Phi under those conditions so Phi Phi will get cancel only one Phi will be there that Phi is always greater than 1, okay ya so this one will be r Ob L square De C b greater than 1.

Actually to be very very specific this is not generally 1 but you can go to the actual curve it will be around 0.2, or 0.3 or around 0.3 okay so then you can also take that one and for example you can calculate what is the diameter for the new particle like you know this is the criteria you want to design the particle, okay you want to design the particle that means you measure you take some particle size and then you have you measure this this and all that, right and exactly you can calculate now what is L square, L square is nothing but your R by 3 if it is a spherical particle so R can be designed and you can say that if I maintain this size of the particle I may not have any R, actually it is not boundary when you draw this actually then you will know that exactly where it starts deviating from 1 all this is 1 know all that is 1.

So that line where it starts deviating slightly less than 1 may be 0.98, 0.99 so till that I think generally this is the general you know as a thumb rule in industry and this was in 1954 so it is most of the time it is only the factor of safety and percentage of errors more (())(28:09) accepted now a says it will not be accepted, right so that is why exact value one can put but this is the idea what they have done and somehow this is called you know Weisz-Prator Criterion but Levenspiel started calling this one as Wagnor-Weisz Wagnor-Weisz and Wheeler Wheeler modulus that is what is the name he has given in his book for same thing this one is called Wagnor-Weisz Wheeler modulus all of them worked in catalysis heterogeneous catalysis so that is why I think he wanted to give like we have LHHW kinetics, okay.

So Langmuir Hinshelwood and Hougen Watson so like that he also says that okay three W’s right there is another you know we also another three W's there is a book not heard which one book (())(29:24) what is the book name, different you say another three W's okay you tell me again I was looking for the whatever he said I was trying to look what are the names he is telling ya what are the names now you told not person’s name oh women, wealth and wine but if you avoid women how do you get children or vice versa, okay women also cannot avoid this is 5000 or 10000 years B.C what you say now I think they will kill you if you say that even wine also will come and kill you ya because even without wine 99 percent of the people on this planet cannot sleep.

What are the other book Welty Wicks and Wilson that is the beautiful book for momentum transfer, heat transfer and mass transfer it is really very good book. In fact you know the mass transfer section in Bird Stewart Lightfoot is not written that well there is lot of confusion, his best part was heat transfer and momentum transfer, momentum is the best in Bird Stewart Lightfoot but in this book mass is the best, momentum is not that good, heat transfer anywhere I think whoever writes heat transfer is okay okay ya that is in between nothing will happen there but I think that Welty book is very nice book Welty Wicks and Wilson very nice beautiful book, okay anyway.

So this is also another name that is given for this modulus and now for a particle I would like to find out what will be the effectiveness factor effectiveness factor for the particle, with this information available can you find out, like a project I will give you I have some catalyst particles and I know what is the reaction you have to conduct, I will ask you to conduct and then ask you to tell me what will be the effectiveness factor with this information available, think.

I think I have to cover a lot and then but most of the time discussion discussion discussion Eta, how do you get Eta Eta Phi square is observable that is that means I know only this see I will (())(31:59) observe means you are may be talking as mathematician or Kavya I know only this is observable for me, okay now using that information that is only information I have using that how do I calculate Eta, think a little bit I say, Anurag.

You will ideas but only thing is you are not thinking, you will definitely get idea only smile teeth showing teeth reflecting more light in the room that is very good, Kavya Kavya is good she thinks like what you tell me you tell me what are these same catalyst only I am talking only about one catalyst I will give you and you have this information right now with you, how do you get me an effectiveness factor Eta, different I am giving you only one particle and then asking you to find out different particles you can do later once you understand, not able to think, how do you calculate Phi Eta also Eta Phi into Eta Phi into Phi where is another Phi coming that means you are restricting yourself only mass transfer as if you have you know you are talking about only this region but you do not know that.

Ya how do you get it that means you are assuming that you are in mass transfer mass transfer resistance regime or the other regime without even doing that you can do that I thought you got the point ya what information you have yes you have then okay in between in between, just one more step thinking correct what you said is right one more step thinking trial and error it work I think because I think there must be one variable also find out no ya you can think I say only thing is somehow you lost interest in whatever you are doing in the IIT Madras academics otherwise you know you can think that is correct.

So Eta I have in terms of Phi, right I simply substitute this Eta here then this all this is measurable then I have now everything in terms of Phi. So now first evaluate Phi once I know Phi then I can go to same equation again and then calculate what is Eta, okay ya I think definitely you are you are very good but only thing is do not you do not apply your mind, okay.

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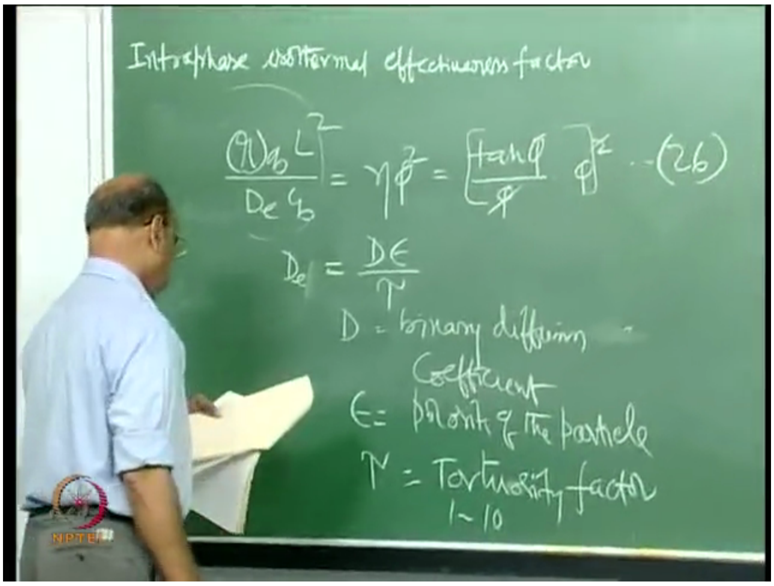

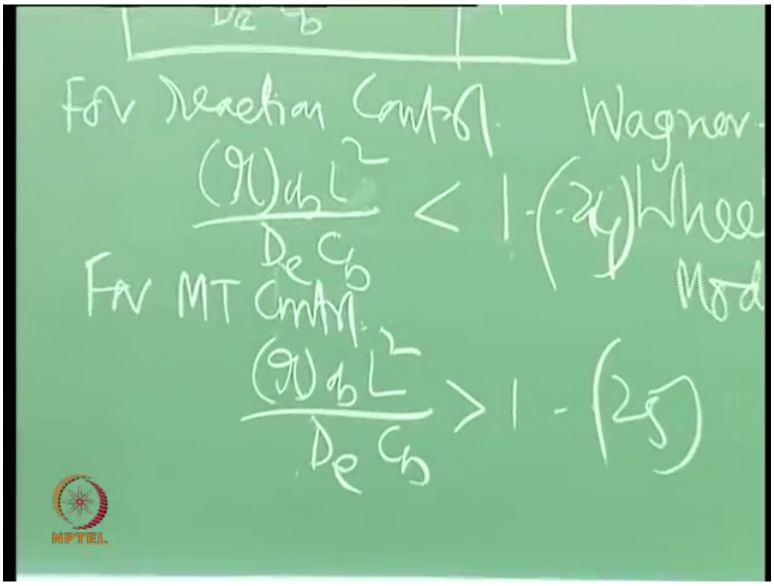

So now if I want to find out what we can do there is r Ob L square De C b equal to Eta Phi square if it is slab for example what is Eta Swami? Tan h Phi by Phi into Phi square so now okay anyway ya so this this can get cancelled and then I have this is the one and this value I know that value may be 0.1, point whatever ya so then I can calculate what will be Phi, once I know Phi, in fact k also you can calculate provided you have some good correlations for De, C b is measurable anyway and there are some fairly good correlations for De and one of that very widely used is the following.

Ya for De effective De this is D epsilon by Tau, okay equation this also I have to write 24, 25 ya same thing I can also write here for example if it is a spherical particle that corresponding equation but only thing is by trial and error I thought when Aruna told trial and error he got the point, okay and Abhinav got the idea Eta substituting the Eta in between regime not you do not have to go to any regime at all now, simply substitute that equation throughout in any regime does not matter so solve for Phi and then Phi and then afterwards you can get Eta, good ya.

So now De effective this is one of the correlations that is used okay where De is binary diffusion coefficient binary diffusion okay I will write here coefficient and epsilon ya porosity of the catalyst particle so epsilon is porosity of the particle and Tau is Tortuosity factor what is the spelling Tortuosity Tortuosity factor, okay and normally it will vary from 1 to 10 that is the scale okay Tortuosity factor, good.

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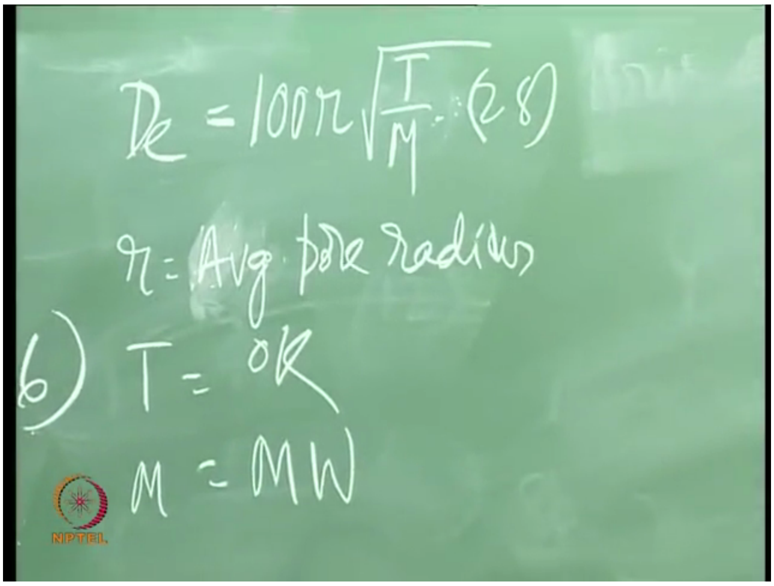

So there is another correlation also that is used for De effective so that correlation also let me write De effective equal to 100r square root of T by M, so this is equation 27, this is equation 28 where r is the pore radius r is average pore radius okay average avg pore radius I think I will remove Aris he is not there anyway recently died, okay ya and T kelvin temperature kelvin and M is molecular weight and I hope you know here binary diffusion coefficients where do you get this data, which book will give you ya Ravi Kumar Ravi Kumar only no ya Ravi Kiran WWW ya where are you from which university Andhara University you have the information with you correct.

Ya so many correlations are available in transport phenomena and there is one book called I think again Bird and (())(41:16) this big book, okay this size book so their properties of many gases, liquids, solids how they are diffusing lots of information this also we should know no it is not that only always you know by the way there is a book called (())(41:30) you know no Kavya how many pages are there 2000 good guess, what is the weight depends on density of the paper ya that is the answer, okay anyway.

So these correlations are available so fairly I think you know that is why even now we do not have data for designing perfectly many chemical engineering system, correlations means it is not perfect, most of the times it is measured automatically there will be some measurement error whatever experiment you do, whatever kinds of experiment you do definitely there will be some error so we have to live with that. So that is why perfect information for designing is not available anywhere for the chemical engineering systems they are very complicated systems, okay good.

So that is how you have to calculate what is the effectiveness factor it is good actually in fact you can join this catalysis centre and you can do the experiments this part they do not know, they are excellent in that Langmuir-Hinshelwood type equation where they can derive and then but they are also testing conducting an experiment that I will tell you after this is over, how do you conduct you know because most of these things depend now on your experimental data, how do you conduct an experiment when you have heterogeneous system, homogeneous system how do you conduct data to find out rate information or information on rate.

Ya only batch reactor all the time, homogeneous means it is the liquid or gas, okay batch reactor or any other reactor but the problem is you know you just follow the concentration and time, right if you are using batch reactor you have to stir very well so that you will not get any any any temperature difference or any concentration difference inside the system. If I have catalyst how do you (())(43:29) catalyst must there inside no if it is a catalytic reaction that is the problem, okay.

Ya that is why we used packed beds and we say that we are using differential packed beds the differential packed bed is only Phi thickness is of particle thickness if it is 3 mm particle size in the laboratory normally we use so 3 into 3 into 3 you know 3 or 5 mm height you put and then that is the packed bed this is the tube like this you put 5 particles height 5 and ofcourse across the diameter and then send it you call this one as packed bed and then try to find out tremendous errors happily you can make lot of errors very happily.

So I think if chemistry people put there they call it is a plug flow reactor because packed bed is plug flow right ya and then they put the liquid phase particularly drop by drop, drop by drop on this catalyst, can you call this one as plug flow? Impossible what should be the what should be the velocity for a plug flow assumption? Infinity and here drop by drop, you can happily imagine what will be the errors in this, okay.

So that is why I think if you join them I think you can do wonderful work there, really doing this work particularly finding out effectiveness factors by the way they are also having lot of atleast as far as I know there are two projects on finding out catalyst I mean designing catalyst, okay this mass transfer and all that they do not do that thoroughly it is not their problem I think they are not simply exposed, okay good.

So this one is over now till now and what we have to now do is that ya till now we have talked about only isothermal, right so non-isothermal effectiveness factors how do we so that means temperature also is changing and you have mass transfer also coming into picture. So in the next class we will try to find out intraphase effectiveness factor non-isothermal intraphase effectiveness factor non-isothermal intraphase effectiveness factor, okay there there are no equations, you do not have any closed form solution like this for effectiveness factor, why you will have definitely a differential equation in terms of mass transfer, you will also have another differential equation in terms of temperature, energy balance and you have another fellow there sitting Arrhenius Arrhenius is always non-linear, okay.

So in these differential equations when that fellow sits there you cannot solve so you have to go for only (())(46:18) okay so that is why we write those equations and then just explain how do you get effectiveness factors and then discuss the graphs what will be the beauty in those graphs, you will have very very nice beautiful information for non-isothermal, okay good I think we will do that in the next class.