

**Chemical Reaction Engineering 2 (Heterogeneous Reactors)**  
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**Lecture 29**  
**Inter and Intraparticle Mass transfer**

In the last class we have done something about temperature gradients, okay which one is important is it interphase gradient or intraparticle gradient by the way which one is which one is important interphase if I ask the question why can you answer why all the resistance for heat transfer lies in film whereas you have almost same isothermal particle that is the main reason conductivity of solids is very very high so whatever temperature is raised there due to exothermic heat or endothermic heat anyway so then immediately it is uniformly distributed in the particle whereas the conductivity of the gas is less so that is why you have the gradient in the interphase, okay film.

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Inter and intraparticle Mass Transfer:

$$(1) r_b = k_g a (C_b - C_s) = \eta k C_s \quad \dots (1)$$

$$\frac{C_b - C_s}{C_s} = \eta \left( \frac{k}{k_g a} \right) = \eta \frac{\phi^2}{Bi_m} \quad (2)$$

$$\frac{C_b}{C_s} - 1 = \eta \frac{\phi^2}{Bi_m} \quad \dots (3)$$

For Control:  $\eta = 1$ ,  $\phi$  is small,  $Bi_m$  is large

$$\frac{C_b}{C_s} - 1 \approx 0$$

$$C_b = C_s$$

Now we will see for mass transfer what will happen, okay again equations are known to you there is no new equation you have to learn and the equation which you have already used one was  $r_{ob} = k_g a (C_b - C_s) = \eta k C_s$ , right this is the balance for overall effectiveness factor, right overall rate of reaction observed rate of reaction, measured rate of reaction so that must be the film and the reaction that is going on inside the particle, right. So ofcourse you are taking first order reaction so this is the rate that is going on multiplied by

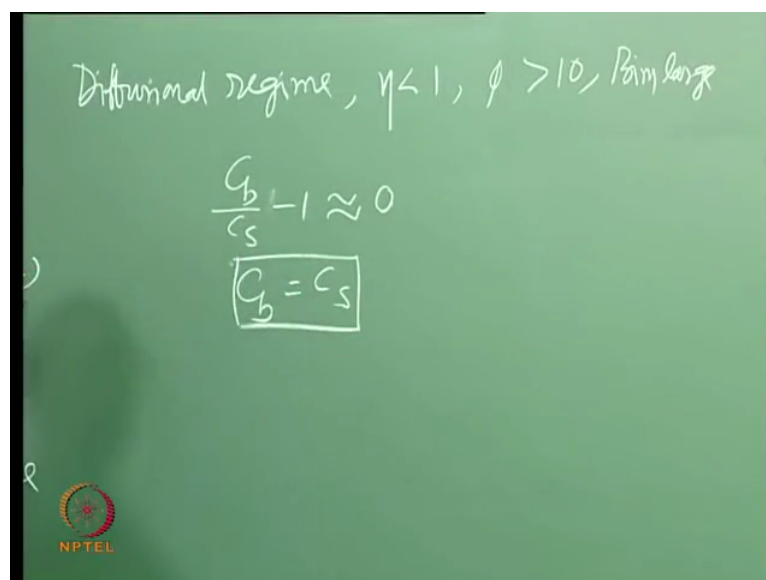
Eta will give me for the entire particle now that is equated to mass transfer because unless these two are balanced you will not have steady state rate, good.

So this equation I will take only this portion so that equation can be written as  $C_b - C_s$  by  $C_s$  equal to  $C_s$  I have got this side  $\eta k$  by  $k_g a$ , okay ya what is this  $k$  by  $k_g a$  already you are experts in this this is nothing but  $\eta \Phi^2$  by Biot number good nice. So that is all I think with this equation we should be able to tell ya this is equation 2 minus 1 equal to  $\eta \Phi^2$  Biot number mass, okay.

So now we imagine first that we are in reaction controlling regime, okay reaction control regime so when you are in reaction control regime what is  $\Phi$  value and what is  $\eta$  value generally in the particles,  $\eta$  equal to 1 and  $\Phi$  very very small and  $\Phi^2$  will be much smaller that divided by Biot number, okay what are the general values of Biot number very high I think you know 10 to the power of 4 so 10000 is the one which you have seen yesterday the other range 10 to 10000 so in between also if you take it will be in thousands.

So that means because  $\eta$  equal to 1 and  $\Phi$  is small  $\Phi$  is small and  $Bim$  large all these conditions will give me  $C_b - C_s$  minus 1 is approximately 0. So what is this  $C_b$  equal to ya  $C_b$  equal to  $C_s$ , okay good. So that means in reaction control regime  $C_b$  equal to  $C_s$  means on the surface as well as ya in the bulk it is same.

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So not you go to the other regime diffusional regime that is mass transfer regime inside inside the particle. So here  $\eta$  is less than 1, right so  $\Phi$  ofcourse large values of  $\Phi$  you will have  $\Phi$  may be greater than 10, okay ya but still when you have  $\eta$  can be even 0.1, 0.01 like

that if you see the graph like this you draw no. So when you go to 100 it may go to even 0.01 I am only drawing in the air, okay you know that one like this it goes like this this side.

So if you take that  $1/\Phi$ ,  $\eta$  equal to  $1/\Phi$  that is the equation, right asymptote. So  $\Phi$  equal to 100 means  $\eta$  equal to  $\Phi$  not so it is very small again. So even here you will and Biot number is large and ya even here you get  $C_b$  by  $C_s$  minus 1 is again approximately 0 Biot number  $Bim$  large, okay again  $C_b$  equal to  $C_s$ . So that means whatever may be the condition inside the particle, okay whether you have reaction control or diffusion control finally you are going to end up  $C_b$  equal to  $C_s$  where  $C_b$  equal to concentration in the bulk and  $C_s$  equal to concentration on the surface.

So that is why safely one can ignore mass transfer resistance through the film, okay I told in a different way we also feel because some of these feelings I think you know we cannot express that clearly but I think whenever you have film and diffusion through the ya pores is difficult than diffusion through the film because it is molecules molecules just going through the film whereas there these molecules have to go through the pores, okay.

So that is why they feel they encounter more resistance than they are colliding with you know molecules in the gas phase so that is also the physical reasoning why we have  $C_b$  equal to  $C_s$  all the time whether you have this regime or that regime and the other one I already explained because gas conductivity is very less, solid conductivity is very high so solid will always maintain isothermal particle, okay.

So that is why when you are actually writing the  $(7:43)$  and energy balances you can simplify automatically many things here because inside temperature gradient will not play a role so you can assume isothermal particle and analyse, only you have to worry about is the external heat transfer, okay how much is the temperature drop from bulk to surface, right and if you go to mass transfer always you can safely ignore film, okay.

So then you have to think about how the diffusion is taking place through the pores that is why most of the time when teachers tell you about the effectiveness factors we always talk about effectiveness factor of particle not external know based on through the film, right but this analysis also Carberry did so beautifully just to say that yes there are many situations where a catalyst need not be porous then internal porosity and all that will not come into picture diffusion through pores and all that.

So everything may happen only in the film so concentrate on the film and also try to find out what will be the effectiveness factors for non-porous particles, okay good. So with all this I think we have thoroughly done about heterogeneous catalysis the basics what we are trying to understand how do you design a catalyst particle in fact you can design a catalyst particle using Weisz-Prater Criterion you can find out that means all of us would like to be in only reaction control regime, correct know that means more amount of mass transfer but reaction is the controlling factor so if the moment you are increasing temperature of the particle, okay the bulk which also automatically reflects there if there is no external heat transfer resistance so you can also increase the rate of reaction, right.

So that is why the always under reaction control regime we would like to operate that is why that criteria tells that you maintain less than 1 then you can design a particle where always you will be in reaction control regime, okay and to be very specific you Cauchy take exact value I think it will come as 0.3 or so for actual one you take that one so that definitely you will be in reaction controlling regime so entire surface area is used for chemical reaction because the catalyst are very very costly so that is why one has to use all the surface and by the way how do you make catalyst? Atleast like small story you can tell how do you make catalyst, why should I have a carrier, what better properties because science and engineering is not (10:49) you have to use very specific reasons

Ya what properties you are talking, first of all why should you take a support, we cannot use straight the catalyst itself. For example iron ore not iron ore for ammonia what is the catalyst, iron right so that iron will be in what form, is there a support for that (11:12) support ya directly why they are not using iron to get active sides, so if I have a porous particle it cannot use active sides.

Let us say I have porous iron particle cannot you make porous iron particle by the way porous iron particle cannot you make no one why it is called sponge iron then why I think (11:50) is telling you cannot make as if God said let there not be any porous iron, one can do that okay but I think in every catalyst there are some other side metals also which will come and you know enhance ya improve the activity of the catalyst, okay that is why it is like cooking where if you are a good cook you can produce a beautiful catalyst, okay really 20, 30 years back that was the one but recently after you try to explain what is happening on the surface where are these active sides at atomic level when you go that is nano technology level then we know exactly what are the active sides, how do you put them and how do you place

them we need a support or not all these things will come into picture they have already come into picture that is why design of catalyst alone is a separate course and the starting point is for example your periodic table from the periodic table you can pick up for some groups you know for some reaction some groups will be very very useful I do not know whether you heard of that or not.

So that one first you have to make and generally I mean there are many many procedures it is not only one method how to (( ))(13:15) of you know because I told that (( ))(13:18) of for example iron on some support, okay or any other catalyst on some support is also one of the biggest techniques where lifelong you have to only get expertise in that particular technique, how do they do that how do they impregnate just think, what salt if there is no salt what do you do, Abhinav

Student is answering: use vapour.

Ya that is also one of the techniques make it vapour allow it flow through this porous support then everything will go and you know it will coat and you have to again ensure that whether only all the pores all filled up with this not filled up the surface area is completely covered with this vapour and then it is one of the you have to take it out and then test again whether you have what is the surface area.

See you have the (( ))(14:23) surface area porous particle if after coating also you get almost the same surface area that means it is almost coated and ofcourse activity also one has to check so there are lot of techniques and another simple techniques are you know precipitation techniques, like you take the catalyst make as a precipitate and then make a powder, take this powder and again compress as a pellet and making a spherical pellet is very difficult that is why even though all the time we draw spherical particle in industry only cylinder because it is easy to make cylinders in the industry for catalyst, why because all the powder you push through the extruders, okay and then whatever pressure you want you can apply and then make the pellets cut, cut, cut, cut now depending on the size what you require what are the normal sizes require or normal sizes that are used in industry it cannot be definitely 3, 4 inches correct no, it cannot be definitely nano particles.

Ya how many microns (( ))(15:29) to see you have gone to industry know, Prabhu you have taken your internship internship where, what did you do there means there is no catalyst catalytic reactors and all that FCC ya that is a beautiful catalyst, SR oils they produce diesel,

petrol and all that. So then I think you have gone to one of the best parts of chemical industry, in fact in chemical engineering developed because of petroleum and all, when petroleum industry wanted more and more information chemical engineering also was supplying more and more information so that is why both group parallel, okay.

So what catalyst they use in the FCC? 2 years ago, 20 years ago I remember zeolites zeolites I think you know these general things all of you should remember I say because every day we are using petrol otherwise you cannot come to the class, how you are using bike, I am not saying you are using bike that means for transportation and all that so you go there and no space at all for any vehicle on the road, how much petroleum how much petrol and diesel they must be using and who is producing all that? Chemical engineers, you have to really lift your collar that because of you transportation is happening otherwise stand still should have been better for the planet, okay because pollution is less.

So like that many things, what you produce so atleast the basic things like petroleum production, ammonium because again fertilizers no food without that, okay because too much population, less area you want to produce more effeteness factor should be increased of the ya land so that is why you put more petrol no not petrol more fertilizers more fertilizers so to produce more and more so again who is producing all that? Chemical engineers, okay so lots of things we are doing.

And I think general things definitely you should remember like when you take a course in reaction engineering, general things like you know what kind of reactors you have, when do you use which reactor, okay what kind of catalyst, what are the general catalytic processes and when do you use fluidized beds, when do you use packed beds he was telling microns, okay micron size Shiv Kumar if you use micron size you can never use packed beds, why pressure drop is tremendous because it packs so beautifully, there is no wide age for the gas to go through mostly gas solid reactions.

So that is why they use fluidized beds, why in fluidized bed you have a freedom of you know degree of one degree of freedom expansion. So when gas enters it pushes the powder outside and then it goes, okay so that is why and ofcourse when it is going it is getting contact with the solids and then you have more ofcourse diffusion, everything is happening there, much more surface area you get in a fluidized bed rather than packed bed but packed bed is still used because design is easy.

So sometimes we do not hire you know not we in IIT we hire the maximum highly intelligent people, okay but some industries they may not require very very highly intelligent people, okay too much efficiency is also bad for them. So that is why they compromise because the people who stay in the industry, who work without questioning because you are more intelligent means more questions, why you have to do like this, you can also do like this all that if you question in industry I think boss says that you stop all those questions because first of all you have to produce, right production is important there and that is why that kind of people are very good in the research side where they can always question and then produce more and more information and for better and better things design, okay good.

So that is why please remember that I think you know how do you produce for example catalyst, how do you design the catalyst now a days I think design of the catalyst with nano technology is going really at very very very sophisticated at atomic level at atomic level people are thinking about how do I arrange these things I mean recently also I saw some of article in nature where to make you know whatever structure you want for the entire particle you can make by bringing 2, or 3 chemicals under certain conditions.

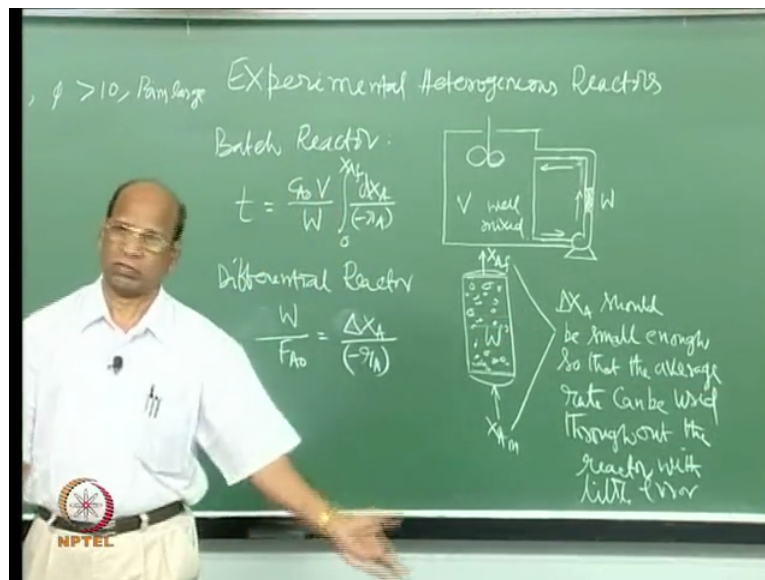
So then it form automatically depending on the charge, depending on the electric field around that and you know they can control the size of the particle, structure of the particle and all that. So that is why nano technology is really helping in customer made technologies I mean customer made catalyst. If you want this particular surface area I can give you you can specify that, otherwise in the precipitation and gel techniques and normal techniques where I have the support also I do not have any choice with the my pores, okay either they naturally occur or when I take the powder and make it as a pellet then I do not have control so if I apply too much pressure then you will have too less pores size pores and if you do not apply much pressure then particle will be crumbling because mechanical strength is not there so all these things are problem but whereas with nano technology wonderful things are happening.

So that is why chemical engineering in which direction it is going means it is going from ya larger size to smaller size, chemist always they reverse they always starts with smaller size, he wants to scale upto larger size. So that is why I always use to tell that chemistry and chemical engineering departments if they are together then this direction they come, this direction we come, both will hit at one point they can straight raise up like Himalayas, Himalayas also have reason of that know is Indian plate mode and then hit that European plate and then raise.

So like that chemistry and chemical engineering together means we can also raise, good excellent okay if you are going to some other new departments start ask for chemical engineering and chemistry to be together wise people would do it but I think we cannot do it we could not do it, okay good.

So this is one and then next one is now all these things like for example this r ob how do we now find out that r ob what are the techniques we have because experimentally we have to also determine that rates we know how to determine these experimental rates for homogeneous systems okay if you have a single phase but here in heterogeneous system we have either fluid and then solid most of the time, right. So under those conditions how do you contact this fluid and solid so that reaction can take place, what kind of reactors we use.

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So that is why we know discuss about experimental reactors experimental heterogeneous reactors ya okay we can also use first of all batch type reactor under even heterogeneous okay but only thing is we have to just see how you know in a batch reactor what happens you put the liquid or gas stir very well so that you get almost homogeneity and take the sample at various times and plot concentration versus time then you get rate and all that, okay.

Similarly for this we can also do but with your own animation you have to do it, so we have a box something like this ya so maybe I have to join this one here ya so somewhere here we will put our catalyst, this is the pump ya it is the stirrer so what we have is it is V inside we have well mixed, this goes like this, like this, like this okay this is the catalyst W you may take 10 grams or 20 grams like that or may be 100 grams and then put it there and you see



now the gas it is a gas phase reaction so always you have the uniform composition here that is why this one and it spends very short time here and then comes because that is why amount is very small there so it comes and continuously circulating all the time it is as if you are stirring the gas okay like in homogeneous reactions.

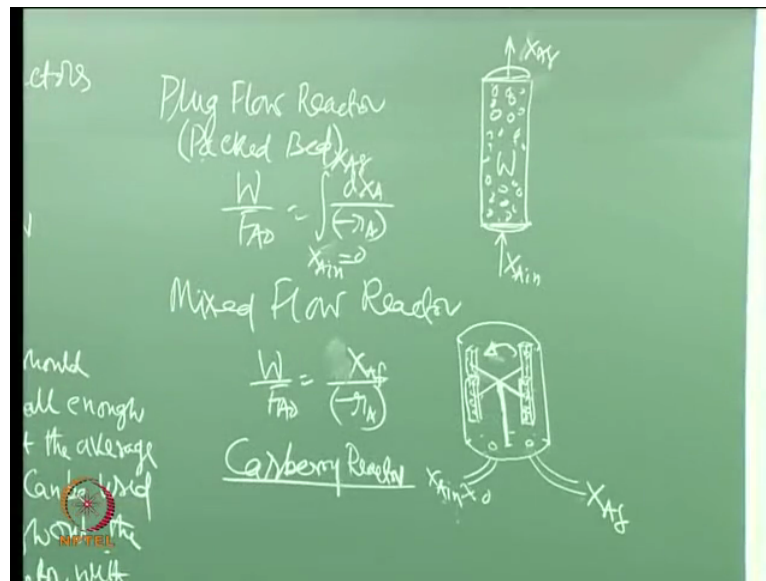
So now we can also use because the equation for this okay I will write here is already known to you  $t = \frac{C_A}{V} W$  is the weight of the catalyst,  $\int_0^X \frac{A_f dx}{A - A_f}$  by minus  $r_A$ , okay that is the equation we just try to derive that if you do not understand you derive on your own because these are the simple reactions, good.

So the next one is differential reactor very widely used this differential reactor is nothing but a plug flow reactor I mean a packed bed where we use our packed bed something like this ya so here we have the packing this is  $W$  ya this is  $X_{Ain}$  that is  $X_{Af}$  ya so here the condition is okay  $\Delta X_A$  okay should be small small enough so that the average rate can be used throughout the reactor ya throughout the reactor but with ya with little error we cannot avoid that error with little ya okay.

So what is the equation we have to use here, here we have to use  $C_A$  not  $W$  by  $F_A$  not equal to (I think I can also need not write this)  $\Delta X_A$  by minus  $r_A$ , right okay this is nothing but your plug flow equation when you integrate this this  $\Delta X$  is  $X_{Af}$  minus  $X_{Ain}$  if you want you can write that  $\Delta X$  anyway I have written here  $\Delta X$ , okay this is the reaction I mean ya but here what you have to see mainly is this is what I was telling you the chemistry will take very lengthy reactor and put a small amount of differential volume you know that is where the catalyst is they put cotton in the bottom, cotton in the top and all that so that you know they can just the liquids or gases can diffuse and then they put drop by drop so you can never use this equation there and they use this equation, okay why this equation is valid only when you have plug flow condition then only this equation is valid.

So that is why I mean it is not their fault but because simply whatever is available in the book if you do it will happen like that only without understanding, right but this is very widely used differential reactors are very very widely used for heterogeneous systems particularly for catalytic gas solid catalytic reactions, okay good.

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So the other one is normal plug flow reactor itself packed bed packed bed so here this is as usual you will have  $X_{Ain}$   $X_{Af}$  integration will not come that is how we are calling differential reactor ya the differentiation of integration is plug flow reactor is CSTR because you are taking that very small I have written here average rate can be used throughout, okay so this is minus  $r_A$  average, okay I will write here average you know how you actually conduct this, you have to maintain plug flow conditions, okay.

So that is why you take small amount of catalyst disperse that throughout on inert particles of the same size okay inert particle of the same size let us say 3mm you are taking. So 3mm of some inert particles but 3mm of some 10 percent or 20 percent of the active catalyst uniformly distribute and then packed bed, right. So from this end to this end you will have only very less rate because amount of catalyst is very very small, there are many ways doing experiment is not that easy I think some of you may be thinking that doing stimulation is great, stimulation any mathematicians can do but experiments only engineers can do, okay ya.

And for example conducting this experiment is not that easy the way we discuss also here. If I ask you complete the design on your own a differential reactor and then do it otherwise I will kill you, okay KK 47 instead of AK 47 okay ya so if you go to KK 47 or if you are afraid of KK 47 then you have to do it right there is no chance, otherwise if it is only exam okay even if I do not do it anyway you will give me D or E I will pass that should not happen, gun should be there then only you will know how difficult it is to do the experiments otherwise

escaping simply escaping because there is another least resistance path, why KK 47 you want still bigger gun, tell me then you do not want to tell, okay anyway.

So that is why I think you know designing this packed beds and then conducting for example we have in our lab because I do always the experiments most of the time we have the biggest problem with the manometers that is why when students joins with me you first connect manometer properly then I will know that you can do your MS or P. Hd ya and what we think you know manometer beautifully written always like this on the board and nicely written delta P, you try to get that delta P in actual conditions I think you know B Tech lab also they cannot get properly because it is already connected, given to them so then I am not talking about them you are also B Tech, okay I mean once upon a time.

So all of I think it is very very difficult for you because it is given already to you so that is why happily we are going opening the tab and then finding out flow rates and all that to finding out delta P and then giving the results, okay so that is why doing experiments is very very difficult and conceiving an experiment is much more difficult that is why P Hd is given for the people who could conceive the you know how to get the data, first of all who can formulate the problem, after formulating whether it is theoretical or experimental how do you really conceive the idea the actual methodology and then next one is how do you analyse the data, same data if I give to X and Y there X may give totally different interpretation, Y may give totally different interpretation, okay without depth very shallow interpretation.

So if you are good automatically you will go deeper and deeper and then try to explain and research is going to deeper and deeper and then bringing something unknown till now that is what is research. So that is why please remember that when you are because all of you are doing some research, some project or other, okay so that is why all these things you know it is not so easily doable here you know the experiments and I think in our department also people think that I mean the faculty who are (( ))(35:22) or students faculty and students who are doing experiments are low funda guys and who are doing the stimulations are high funda guys, high funda, low funda, delta C ya it is everywhere I mean because I know here so I am just thinking I am telling you it may be everywhere but I think before the computer you can stimulate many many things but actually go to the lab and try to get 1 millionth of what is stimulated, try to get on your own then you will know the difficulty, okay.

First of all you have to go and request many times so that (( ))(35:57) that is the starting point you know mechanics okay starting from mechanics, starting from lab attenders, starting from

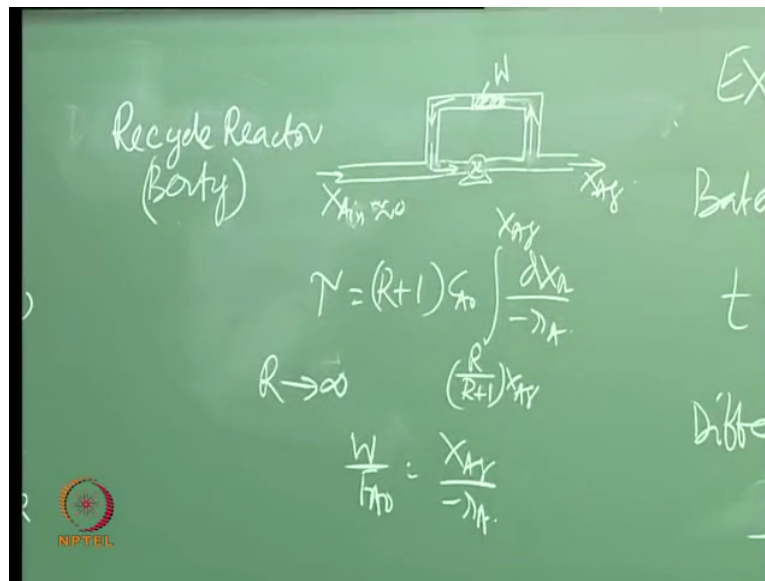
sweepers everyone you have to handle computer what do you handle only you handle yourself, okay and make noise tick tick tick tick tick tick so that is all what you do there, okay anyway good.

This is plug flow reactor where we have the equation already here  $C_A$  not I will write here I will write here  $W$  by  $F A$  not now Swami what you are asking is  $X_{Ain}$  normally which is 0,  $X_{Af}$   $dx A$  by minus  $r A$  this is the actual plug flow reactor where there is lot of variation from here to there, whereas here it is as you said correctly it is mixed flow throughout the system we are imagining that we do not have much difference in the conversion but that small conversion is because of certain rate, okay that is what what you have mentioned, okay.

So the other one is mixed flow mixed flow reactor this mixed flow reactor was design by Carberry so what he did was he has taken a box, a cylinder ya so something like this ya so those are the poles there then so as a rod ya so here you have a box and here again you have another ya so it is actually 4 boxes you know these are the mesh boxes so they fill up the catalyst here okay and then ya rotate, okay it is very nice so here it is  $X_{Ain}$  may be 0,  $X_{Af}$  so the gas goes inside this is rotating so the gas goes and then contacts there and anyway continuously you are pumping and then here definitely outlet is open so then it will come out here  $X_{Af}$  you measure this, you measure this normally this is 0, okay and the equation for this  $W$  by  $F A$  not equal to again  $\Delta X$  if this is 0 that will be if this is 0 that will be simply  $X_{Af}$ , okay if this is 0 that will be 0 I think let me write that so that you will have atleast one ya this expression, this expression is familiar to you, okay good.

So the last one ya this is Carberry reactor, okay ya this is one of the easiest reactors directly you can get but anyway it is not that easy also to imagine because when the gas goes and then when it is moving with the solids, okay because solids are rotating like fan and gas also moves the relative velocity between the between the gas and then solid is how much 0 or more because gas also moves with the same speed as solids so what is the relative velocity? 0 that is not good for the mass transfer to take place, okay right so that is one of the difficulties but still that is one of the techniques they use there.

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So then you have the recycle reactor this reactor was designed by Berty Berty was a professor of chemical engineering somewhere University of Akron Akron University of Akron, okay. So here it is normal our here I have space ya so that is like a fan inside ya  $X_{Af} = 0$  so here so this is catalyst  $W$ , this is also coming ya so some amount of gas is recycled some amount of gas is recycled so here, right so that depends on how much you open here so depending on this opening remaining will go there, this you can adjust so recycle ratio you know amount removed by total amount recycled that is recycle ratio or so this we have done already so the equation for this is  $\tau = R + 1 C_{A0} \int \frac{dX_A}{-r_A}$  by minus  $r_A$ , okay.

When  $R$  equal to 0 then you will get this equation, when  $R$  equal to infinity both can be done here this is the advantage of Berty reactor so depending on recycle ratio you can operate that as either plug flow reactor or mixed flow reactor. So when  $R$  equal to infinity because when you are doing experiments it is always better to have directly getting  $R_A$  like this that is the advantage here also directly getting  $(\frac{R}{R+1}) X_{Af}$  again integrating and all that so that is why if you are able to maintain  $R$  equal to infinity mixed flow condition you get the same equation as  $W$  by  $F_{A0}$  not equal to  $X_{Af}$  by minus  $r_A$ , good.

So these are the reactors what we have and there are many other reactors for example it is not that easy again to go to you know catalytic non-catalytic reaction like for example if you want to find out iron ore kinetics, how iron ore is getting converted to iron and if you want you have to again think, if you are trying to find out the kinetics in gas liquid systems again you have to think what kind of reactor you have to use.

So that is why chemical reaction engineering fundas are very very high because each problem is separate problem to be (( ))(46:11) so then you have to really imagine how to conduct experiments, how to analyse the data, okay how to develop the models for that kinetics like you have seen Langmuir Hinshelwood kinetics that is different and you have also seen non-catalytic reactions like shrinking core model, homogeneous model all this.

So that is why each reaction is a separate one and we have three phases and combination of these three phases will give you really help, can be liquid-liquid, gas-solid, gas-liquid and all that you know ya solid-solid much more help so all these reactions, good. So with this I think you know I have closed the entire catalytic reactions so now what we have to do is in the next class packed bed reactor design, we will have some equations I mean some models for packed bed design and then we will take some simple problems and then I will ask you how to design that, okay good.

So Monday I will not be there, so you will be happy you are free, you can prepare very well and Tuesday we have examination MS, P Hd students you can sit in the same room like last quiz 1, okay 255 I think you said 355, 355 you said.