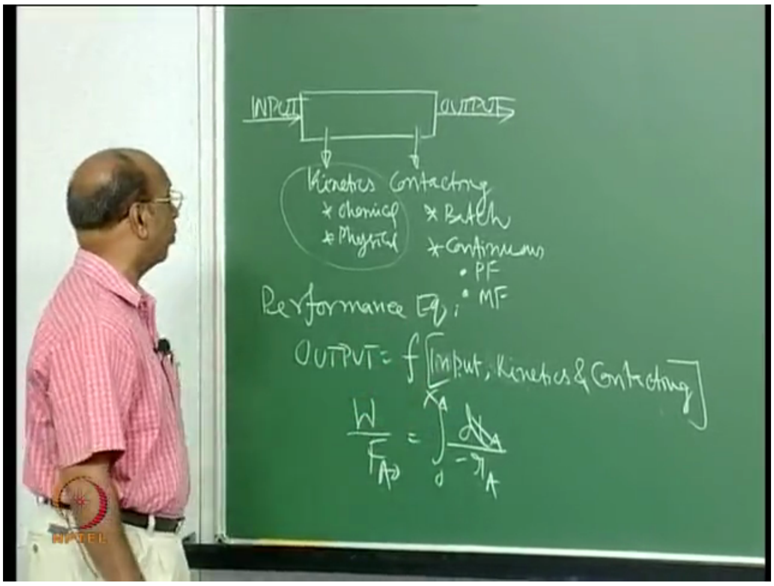
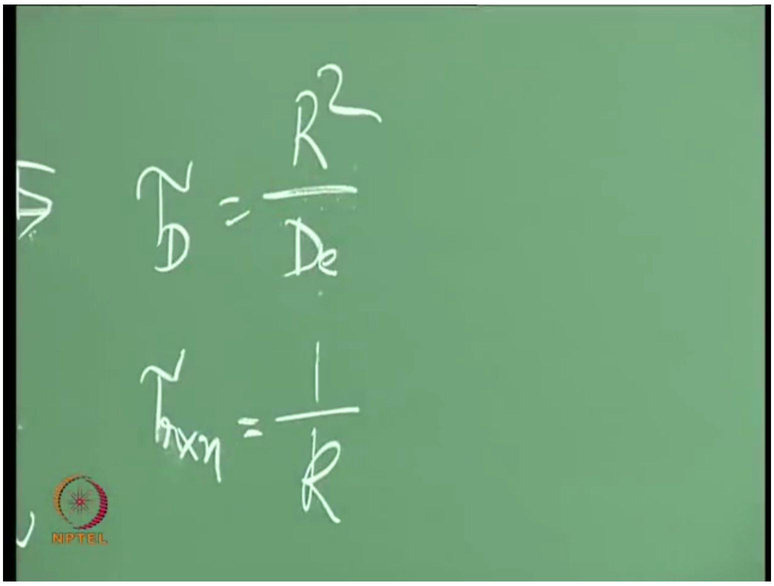
Chemical Reaction Engineering 2 (Heterogeneous Reactors)
Professor K. Krishnaiah
Department of Chemical Engineering
Indian Institute of Technology, Madras
Lecture 30
Packed (fixed) bed catalytic reactor design

So till the last class we have discussed about the reaction rates we started with at 7 steps, we started with adsorption desorption surface reaction that is the pure reaction rate without any mass transfer and heat transfer coming into picture, then we have taken interfacial gradients and intra facial gradients and then finally now we have a rate expression.

(Refer Slide Time: 0:43)



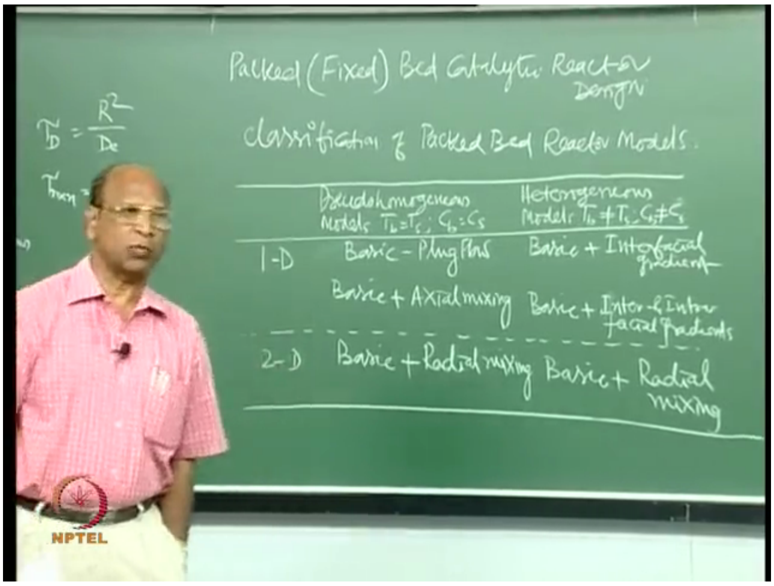


So if I go back to my original diagram which I have been drawing all the time that is ya kinetics all that we have come there so here we have input, output, kinetics, contacting, here we have chemical, physical, batch, continuous and then we have PF, MF all ideal contacting, then the performance equation, equation output as a function of input, kinetics kinetics and contacting ya this equation also we have seen. What we have done was this one thoroughly entirely for the heterogeneous catalytic reaction.

So here we have kinetics I mean for design finally you need the input which all of us know how to find out, kinetics which will give you minus rA and then contacting what kind of reaction you are going to take and fortunately for us in a continuous system we have only two most of the processes are only continuous and then that is why these two reactors one of them you should choose and contacting will give me type of reactor, kinetics will give me the rate and that rate only thoroughly we have done using chemical and physical aspects. Chemical aspects is the intrinsic rate what you have derived for using Langmuir Hinshelwood Kinetics, okay that is minus rA ofcourse even though all the time we will say only first order reaction but it can be any order or there is no order at all for most of the reactions so this entire thing will give me minus rA, okay.

So now if I take for example the packed bed reactor where it is a plug flow reactor then the equation for designing packed bed is this in terms of W, where W equal to weight of the catalyst 0 to X A dX A by minus rA, okay this entire expression is due to the contacting pattern, right and in this expression I have minus rA kinetics and in this expression I have input the F A not, okay.

(Refer Slide Time: 4:06)



Packed (Fixed) Bed Catalytic Reactor Design

Classification of Packed Bed Reactor Models.

	Pseudohomogeneous Models $T_b = T_s$; $C_b = C_s$	Heterogeneous Models $T_b \neq T_s$; $C_b \neq C_s$
1-D	Basic - Plug Flow	Basic + Interfacial gradient
	Basic + Axial mixing	Basic + Inter- & Intra facial gradients
2-D	Basic + Radial mixing	Basic + Radial mixing

So this is what now we are trying to we are trying to do now next few classes that means we would like to have ya we have to design using this information the packed bed reactors, or fixed bed reactors, right packed bed reactor or fixed bed reactor I do not know which one you like, you like packed bed reactor or fixed bed reactor, which has got more meaning? Pack why catalytic reactor design.

Ya why do you say packed bed packed bed is better than fixed bed? Just like that is there any meaning for packed bed and fixed bed? Ya packed bed tell me ya again more correctly if you say fixed bed is the correct one because bed is fixed bed is fixed atleast between two two plates distributers otherwise it can fluidized and the entire bed also packed bed also can move, right entire packed bed can go up that is what what we call moving bed and it is called entire bed, so fixed bed is the correct word even though many times we say packed bed, packed bed, packed bed, okay good.

So now for the design of this you can go to any level whatever you want, okay I will just describe one I think nowadays one of the new subjects or the future of chemical engineering people say I also believe that is multi scale chemical engineering multi scale, right. So multi scale means you have to start from the smallest may be from nano or less than nano too to the almost to the planet level and planet level.

So that means almost chemical engineers are associated with molecular level to planet level. So I can give you the example for example taking catalytic reactor packed bed reactor itself what is the starting point for us? Starting point for us is the chemical reaction which occurs at molecular level. If it is a catalytic reaction then you will have a catalyst that catalyst you have to prepare, how do you prepare catalyst again various techniques we have discussed may be crystallization one of the techniques and if you take one specific example like zeolite zeolites can be made beautifully through chemical reactions, whatever structure you want you can get it depending on what kind of reaction you are going to conduct that means you can control the structure of pores using zeolite catalyst, for many other catalyst it is still it is not possible to have that kind of structure, okay.

So then if I have a particular structure known to me and also my molecule size known to me these two, so I will take a zeolite catalyst with some pores zeolite crystals for example it is not even pellet zeolite crystal I have to make first these crystals have the holes the pores so that pore naturally should be slightly larger than the pores larger than the catalyst sorry the molecular size, okay.

Now what happens if you are theoretically if you want to theoretically find out how many molecules are getting diffused you have to go to quantum mechanics level because these molecules are driven by thermal forces at molecular level and because of these thermal forces the molecules will vibrate, translate and rotate, right. So for example you have to find out the speed of these molecules how they are going and entering through the pores, if you want to calculate the rotational speed, okay then you have to use the Schrodinger equation to find out or even just before that if you temporarily assume that there is no catalyst there then you have the kinetic theory of gases and at room temperature you know that Bird Stewart Lightfoot also has given this value I think you can calculate also that 200 meters per second at room temperature the molecules can move according to kinetic theory of gases, they are moving in this room also with that same speed but only thing is we are not able to see, okay.

But when you are having more and more molecules that means dense gases then what happens this free flight you see at what level we are discussing the free flight of individual molecules are restricted because there are many abstraction because other molecules are there, it is like I do not know whether you are experience at this I have also gone long back 20 years I have gone now it must be worse, there is a street in Chennai called Rangnathan street Rangnathan street have you gone to Prabhu you would have gone, okay that is what is highly dense packed bed, okay you cannot move you have to really make effort to go through that packing.

So when you have that kind of so many molecules very close the free flight of this individual molecules will simply become the phenomena of diffusion, otherwise that is why kinetic theory of gases is for more number of I mean the less number of molecules per unit volume dilute gases for example, if you go to very very dense gases then the free flight of the moment of the individual molecules will become diffusion that means it has to fight to diffuse through the other molecules, okay that means diffusivity coefficient will automatically come there and Schrodinger equation will automatically come there because you should find out the orientation of the molecule that means rotation and all that so that the molecule should properly orient to go into the pores otherwise the molecules particularly when you are talking about our catalytic cracking then you have the long chain molecules, long chain molecules when they are moving in this direction they may not enter, chain is in this direction so they have to rotate in this direction and then try to enter through the pores that is why in zeolites most of the time I have told you you know three types of diffusion, right what are those?

Knudsen diffusion, Bulk diffusion and Configuration diffusion and the speciality of configuration diffusion is that the molecule is always in touch with the surface of the catalyst and whereas the bulk diffusion it may not be even seeing the catalyst surface that means the pore wall, whereas Knudsen diffusion Knudsen diffusion, what is the size of the pore for Knudsen diffusion? No we have talked this about in mean free path ya if the pore diameter is almost around 5 times the mean free path of the molecules in kinetic theory of gases then you will have the Knudsen diffusion but our idea should be to go for configuration diffusion, why because each and every molecule should easily see the wall because reaction is happening on the wall.

So when the molecule goes and gets absorbed there is surface coordination between the molecule and then the surface then because of the energies involved bond energies some of the bonds will be loosen they are broken then the molecules will other molecules you see all this is at molecular level and we never bothered to know all this 50 years back because what is that I want there I have a catalyst, send the gases analyse the gas find out how much is coming.

But now because of the efficiency you know to improve the efficiency this level also people are thinking that is one scale nano scale sorry I think even less than nano scale around nano scale only all the phenomena what I have described. So now you have the pore and through the Schrodinger equation and also kinetic theory of gases you can try to find out how the molecules oriented and then trying to diffuse into the pore.

So now diffusion automatically comes there because it is configurational or Knudsen or Bulk because most of the time we would like to be configurational diffusion because surface area should be always in touch with the molecules or vice versa, right. So after that then these catalyst crystals zeolite crystals you make them as because crystals as it is I cannot use in the reactor you have to make them as pellets, okay.

So now these pellets may be of 3mm diameter or 4mm diameter, 5mm diameter, right. So when they are making this one as 4, 5mm diameter then the diffusivity will come automatically into picture that means you know Thiele modulus, right. So that means what is the total surface area now I know how to calculate at individual molecular molecules level and then pores or individual crystals, now all those crystals came together as a particle, right.

Now I have to say yes now what is the diffusion that is going through this and there is a beautiful definition which I have I think it did not occur to me at that time to tell you the bigger the particle you will have more time for diffusion, right I mean it takes more time for diffusion and that is why there are two times involved diffusion time and reaction time, which one should be large and which one should be small? You have two times diffusion time for the molecules to diffuse through the particles and reaction time for the reaction to happen, which one should be smaller ya if you are able to make diffusion time much much smaller than the reaction time that means all the surface area is already used I mean it is being used by the molecules.

So now that is the thing, in fact the ratio between the ratio between diffusion time and reaction time is nothing but square of Thiele modulus I will just explain, diffusion time I think I will write here diffusion time Tau D is R square by D, where D is the diffusivity, R square is the radius of the crystal okay when it is diffusing through, okay or the particle, right okay and Tau r reaction time for first order it is very easy to remember how do I find out Tau r for first order reaction time, I am not talking about integral CT and all that.

What are the units of k? Time inverse so that is the indication of first order reactions this is the time, this is seconds here also I have seconds because this is meter square per second, meter square there. So the ratio between these two tell me is it Thiele modulus Tau D by Tau rx ya Pi square Pi square that is the beautiful definition again this I did not occur to me when

I was discussing earlier, okay so this is wonderful that means you should always try to have you know always effectiveness factor 1 means the Phi should be as small as possible, okay good that is nice.

So that is the level what you are talking and then now you take the particles and let us say 5mm particles so is it important whether to have 5mm particles or 10mm particles or 20mm particles is it really important to know what is the size, why? Diffusion time because that means there is a some optimal particle size that is as far as reaction is concerned, there is another thing also again particle size that comes when I am now talking about the reactor because we have the molecules, crystals, particles now you come to these particles are putting the reactor level in the packed bed reactor.

So when you are putting in the packed bed reactor what is the use of particle size I mean will you use that in calculating any other parameters for reactor size, pressure drop Ergun's equation so if it is too small pressure drop will be very large, okay if it is too large then diffusion time is large so somewhere you have the optimum that is coming at reactor level, right.

So once you have the reactor design properly this reactor is kept in the plant level correct know we do not have only reactor alone even though that is my dream that you know only reactor dream dream dream reactor okay dream flowchart where you have only reactor nothing else that can happen only when you have reaction at room temperature, 100 percent pure reactants, 100 percent conversion, atmospheric pressure, or the reaction is happening then whatever you have is pure reactant is coming into the reactor and then pure products coming out, straight away ya storage stand to super market straight away you are sending the material to the super market then they can open the tap and sell and sell to you wonderful wonderful if that is really possible.

But currently that is not possible so you have the reactor along with the reactor you have so many other equipment that is plant and if you see the molecular level is nano level, okay and then particle level is micro level, okay and then the size of reactor and then plant is at macro level plant also you are checking know then definitely we know chemical engineers are the main people to pollute the atmosphere in many cases, okay.

So that means the waste gases from the plant going to the atmosphere. Now you have to model the atmosphere to understand how the dispersion of pollutants you see know molecules to plant level, but fortunately all the gases are only not able to leave the planet but it is only within the atmosphere of the planet, if that is also throwing away material to outside to some other planets then it will become universe level.

So those are the scales chemical engineers are working appreciate atleast now and lifelong you can have your entire research based on only molecules and Schrodinger equation that is your research area that is all and some people can concentrate only on the Thiele modulus, okay Thiele modulus means you know again intraphase gradients, interphase gradients and all that, some people can spend all their life only to develop Langmuir Hinshelwood Kinetics that is all throughout their life.

So similarly some people can also concentrate only on the Ergun's equation since Ergun's failed in the P Hd examination and when he first told about that equation and that is what the story someone was telling me some UK professor he know that Ergun has been failed because there is no theory in that it is only empirical correlations, correct know Ergun's equation is only empirical correlations where they have two terms one is (())(19:49) term and the other one.

So it seems after doing that work and then he submitted that one as the P Hd thesis, examiner can throw that thesis out no theory only empirical so no P Hd for you and that is the equation what we have been using all the time I think on this planet wherever there is a packed bed, same story with Monod's equation also that was also first not accepted by the general I do not remember that general it was rejected by the general Monod's equation, not Monod's Michaelis Menten equation Michaelis Menten equation because that mechanism and all that many people did not know at that time so that equation also was that paper was rejected but afterwards it was accepted by some other general and then you see everywhere without Michaelis Menten equation and Monod's equation both are similar know except one is for axioms, the other one is microorganisms both are same.

So I think now everyone talks about in fact entire biochemical engineering only two equations correct know what Savita ya only thing is you add some kind of deactivation terms what is that called deactivation or inefficient terms and all that for the reaction to take place so these are the scales we are talking. So when you talk about packed bed catalytic reactor design what level we are talking, we are talking about only reactor level but before that and after that there are many many things, okay.

So that is why that story I thought I will tell you, so for packed bed reactor design alone again if you take okay I will let me concentrate only on that scale reactor scale, how many ways you can design, okay taking the entire system as simply plug flow reactor ideal plug flow nothing else or otherwise you can take this one as axial dispersion correct know because that is the nearest non ideality, okay and you can also take radial direction then it will become two dimensional model because variation along the length of the column, variation along the ya diameter of the column which is true many times because particularly when you have and we are talking about heat and mass transfer together it is not no more isothermal, okay we are talking about energy balance and heat balance because temperature profiles as well as concentration profiles both are important for us so radial direction and axial direction all this what we say is for pseudo homogeneous models, what do you means by pseudo homogeneous models I do not know whether you heard of this or not, pseudo homogeneous model for packed bed reactors ya what is the meaning actually ya axial direction why do you call that is pseudo, what is pseudo that is one dimensional, what you are telling is if I say one dimensional I am not bothering I simply do not care what is happening along the cross sectional area, okay ya what is the meaning of it right right equations are similar to homogeneous models but what is the meaning that is why you are calling pseudo homogeneous model. In a packed bed what is the imagination when you say pseudo homogeneous, what Abhinav.

So ya very close then why do you call it is pseudo homogeneous, what is pseudo homogeneous it is not actually but on what conditions we are saying that you know this can be pseudo homogeneous ya Anurag just I want you to think that is all it is not that I am trying to because before I give the answer so that means what is that you are trying to because there is a catalyst ya very close but I think still you can tell, simply we do not feel the presence of solids (())(24:33) as he said bulk properties alone when you take the bulk properties alone and then try to find out the actual conversion along the length if it is only 1-dimensional model that means simple plug flow, okay when you have that situation we say we have pseudo homogeneous which is very famous in industry because we do not have to bother about what is happening in the particles, right how do you take care of that you already have that because is particle whatever happening inside if you are not able to find out exactly right multiply by Eta, okay effectiveness factor. So you are making converting that into anyway bulk rate so that is lot of amount I mean large amount of data available on pseudo homogeneous models that is one section.

So then you can also use heterogeneous system heterogeneous model in heterogeneous models you always treat gas as gas or fluid as fluid and solid as solid. Now you can imagine solid is one part all liquid is another part or fluid is another part now you have the concentration gradients in the liquid, okay and also in the solid. If you again assume that at any cross section you have perfect mixing of the liquid then you have horizontal some concentration here and then when they touch the solid then you have the gradient inside the solid, temperature also same, okay that is in one direction may be you can do this only in axial direction where the temperature and concentration gradients are existing within the particle.

So now what you have to do you have to first solve the concentration and temperature gradients within the particle, then you come to the surface and if there is interphacial again again solve for surface and then through the film through the bulk and now you come to the bulk write the equation in term based on bulk, so you have to first solve the particles for temperature and concentration.

You know what are the equations you have to use, question number 3, number 3 or 4, question number 4 same equations so you will find out now T and Ts depending on the boundary conditions then from Ts to Tb same thing C to Cs and Cs to Cb now once you have Cb that is where the plug flow is happening in the axial direction or you may have the generally we do not take axial mixing and all there because the mathematics will be very very very complicated so normally we assume that we have plug flow but consider the temperature and concentration gradients along the radial direction sorry along the axial direction and all sort for two dimensional radial direction but two dimensional heterogeneous models are very very rare there are few only few academicians have tried to solve those equations.

So that means what? When you are solving this interphacial and intraphacial gradients you assume that at any cross section if you take one particle and then able to write the equations throughout it is same that is what is the assumption. So along the radius so in the two dimensional model is that it is not uniform, if I simply solve only one particle and then assume that throughout it is same it is not correct because there is also concentration and temperature gradients along the radial direction not only in this direction, okay that means if I have the temperature in the radial direction each particle will have a different kind of you know there is a temperature and concentration gradient there otherwise one line and over that you have axial mixing or you may have simply plug flow that is all what we have.

So these are the possibilities what we have and I will also write that for your notes otherwise I am sure you will not remember anything, okay absolutely you do not remember because what is your interest it is not coming in the examination because normally I do not give this kind of theory, okay that is what your expectation but I can also give anytime, okay.

So that is why let us first write these models and then we have to go to the corresponding equations ya classification of packed bed I am using packed bed only reactor models. So let me here we have pseudo pseudo homogeneous models where we take Tb equal to Ts, Cb equal to Cs then we have heterogeneous models Cs good. Let me take 1-D first 1 dimensional or the simplest one is ideal or okay basic basic is plug flow because for packed beds do you know why we are taking for packed beds plug flow, right that is the one and okay let me finish this first then we can go to heterogeneous systems.

Then in the same thing I can also have basic plus axial mixing it is still 1 dimensional correct know you have plug flow over that you have axial mixing but all the changes only in the along the length of the reactor so this is the one then we have 2-D basic plug flow basic plus basic is plug flow plus radial mixing, okay basic plus radial mixing, right basic will tell you variations along the length and radial mixing, okay.

So when you come here for heterogeneous okay let me also draw this boundary somewhere there ya here you have basic interfacial gradients and in the next again 1-dimensional this can be basic plus intra and interfacial, inter and inter and intra facial gradients, good. So here basic plus radial mixing also taken into so these are the general things what we do, okay and we are always that means we are always trying to tell that in a cylinder most of the time we use cylindrical part cylindrical reactors, okay packed bed, why why do not we use square cross section or rectangle cross section because distribution is not proper, distribution in the corners and all that you will not have proper flow that is the reason and because we have that symmetry so that is why we will take only 2-dimensional but you not take this direction because cylindrical also will have r theta know that one we will not take because of the symmetrical diffusion, okay good so this is the one.

And based on this now I am not going to say anything about this accept may there is time I will write one or two equations how do you write those equations that is all and those equations are already known to you because for separately plug flow you have to write and separately for particles you have to write and combining them is your Ts boundary conditions at boundary what happens, okay all these equations are known to you but only thing is you have to bring them together, may be as an example I will show you one set of equations for solving but anyway or this course you do not have to really worry because they are really very very complicated models but course is not writing for the examinations, courses is a preparation for your future model, okay that is why most of the time because you are not going for chemical engineering you are not carrying the chemical engineering subjects, okay.

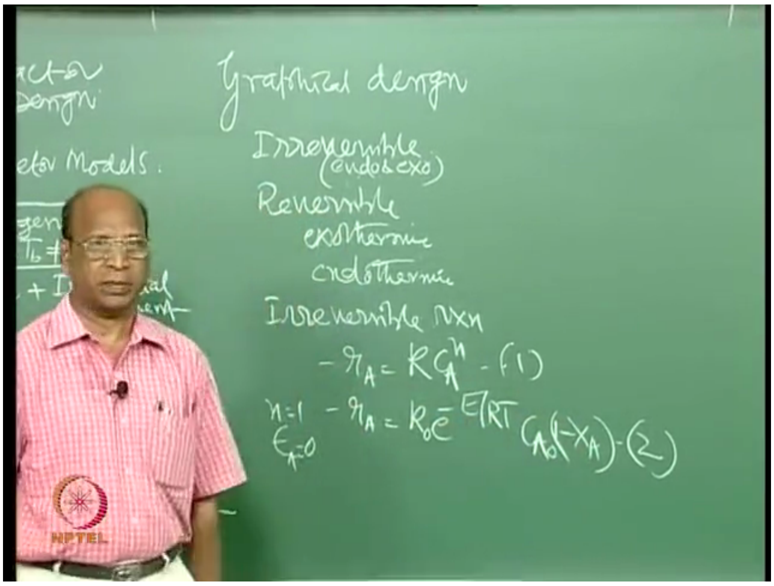
So that is why unfortunate things are happening you know in this country where we do something and finally end up doing something else, totally something else, unconnected, okay. So that is the reason why but anyway as teacher I cannot assume that and keep quite because I do not have to teach you at all if you assume that anyway you are not interested in chemical engineering so that mean that I have that attitude then you do not have to I do not have to come to class you do not have to come to class, okay.

So that is why I cannot assume that so more amount of time we will try to spend on pseudo homogeneous models and I will give you one or two set of equations for you unfortunately in future if you become a chemical engineer dealing with atleast you will remember that okay I think I know this somewhere, he may not know who thought you who may not know which subject but still memory you know sometimes it will come that neural connections when suddenly something happens so lot of chaotic theory in brain is also there in brain suddenly some connections will come, okay.

So one of those connections may tell you that may be I saw this kind of equations somewhere so that is the reason why we have to do this and a little bit of this, okay and before that I have some other passion for my design without writing equations how do I design the reactor, okay this is graphical design you need some equations but not solving differential equations, here differential equations automatically come because packed bed is a distributed parameter system, okay so that means the changes are occurring along the length, okay.

Whereas if the same thing if I want to write design equations for mixed flow reactor than you will not have differential equations but you will have algebraic equations that is the main difference between distributed parameter system and lumped parameter system, okay so this I think you should know each one of even if you not becoming chemical engineer also you have to note this system because that will automatically differentiate the type of mathematical equations what you are trying to use, okay right good.

(Refer Slide Time: 36:52)

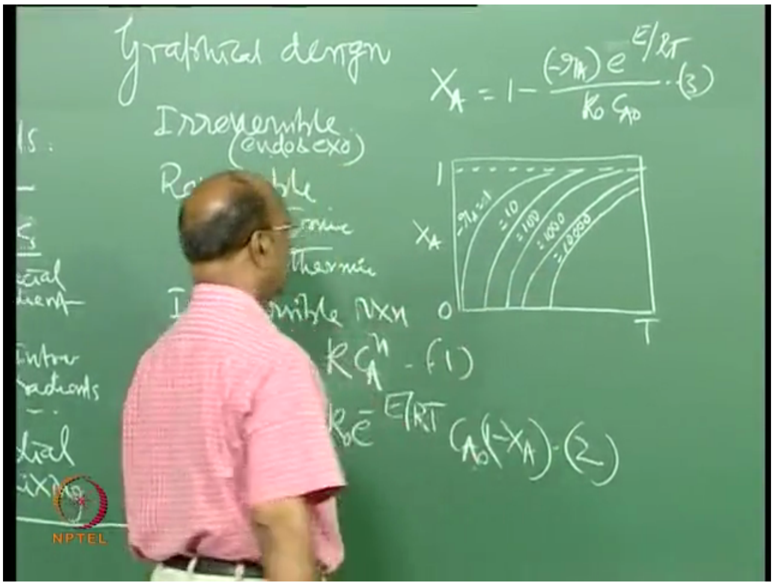


So and with minimum amount of mathematics how do we actually design this is the graphical design which I have done something in the last semester reactor theory when you are talking, okay. So our reactions we will say that we have irreversible, reversible exothermic and reversible endothermic, here does not matter reversible endo, exo both are here endo and exo, okay good.

And for reversible reaction I have an equation now may be irreversible irreversible reactions a general order if I take I will have minus rA equal to k CA to the power of n as usual I am going to take n equal to 1. So this is minus rA equal to for n equal to 1, okay this becomes k 0 e power minus E by RT C A which is nothing but C A not into 1 minus X A that means I am also assuming epsilon A equal to 0 this again we like to simplify the equation procedure is same exactly same even if you put epsilon also does not matter, even if you put second order also does not matter I think it is the same procedure procedure is same.

So now there are three things for me I have minus rA minus rA is one parameter, T is another parameter, X A is another parameter I have T, X and minus rA. So now I can make plots using anyone of them Y and X, X and y the other one will be the other becomes a parameter, okay these two are variables, good. So the other things are constant because k 0 I know frequency factor E R is the gas constant and C A not also I know initially.

(Refer Slide Time: 39:30)



So when I write this equation in terms of okay let me write here X A I am solving equation 2 this will be 1 minus minus rA e power minus E by RT plus RT by k not C A not so this is equation number 3, okay now I can plot this particular graph as the convenient way as I told you any two parameters can be chosen here, third parameter will be automatically there, okay so but most convenient for design is X A versus T and rate will be the parameter.

So it is a irreversible reaction so maximum conversion will be X equal to 1, X equal to 0, okay T we cannot say anything. Then if I assume a particular minus rA let us say 0.001, 0.01 that values we cannot say but you have to start from the lowest to the highest and you have to start for specific reactions some specific values this is only by trial and error you should get otherwise there is no universal law there.

But anyway minus rA equal to 0 means what? Equilibrium, okay but here there is no equilibrium because it is a irreversible reaction, right it is not reversible reaction so that is the other extreme, right. So but minus rA very very large value I can start it is a very small value I can start I can go to large. So then you will get curves like this all of them tending to 1 all of them tending to 1 this is for example minus rA equal to 1, 10, 100, log scale I am going 1000, 10000, okay they may touch here also this is one set okay shall we stop here Shekhar run, okay we will stop here.