Chemical Reaction Engineering 2 (Heterogeneous Reactors)
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Lecture 01
Introduction to Kinetics (Gas solid non-catalytic reaction)

Ya and (())(0:11) systems also for example the first one what we discussed was the gas solid reaction, right ya.

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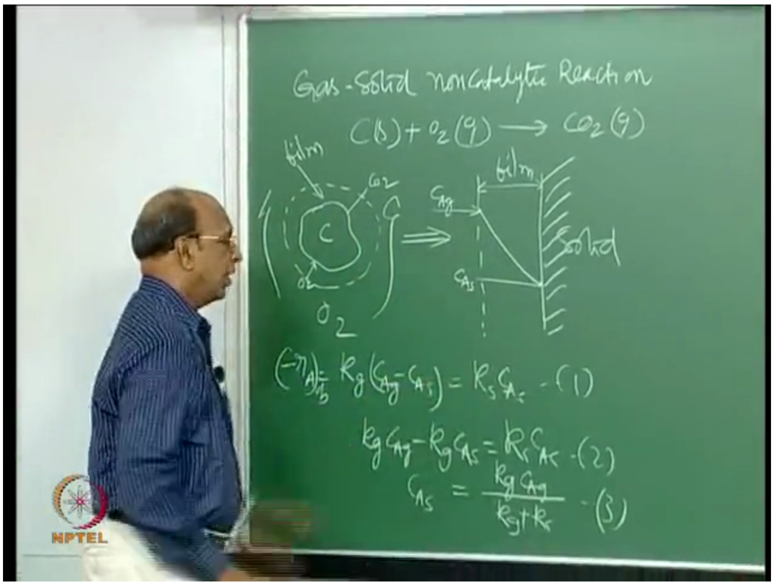

So gas solid non-catalytic reaction, right. So the example which we have taken was carbon solid plus O 2 gas giving us CO 2 gas and the model imagination is something like this so we have solid, we have this is carbon, then we have film and all around we have O 2 and O 2 has to diffuse to the surface and CO 2 has to come out and we have also written the equations like ya this also can be modelled like this as solid, this is the film, right gas film and then if I draw the profile this is C Ag that is the concentration of oxygen in the gas space then I may have something like this, this is C As, right.

So at steady state conditions the amount of oxygen which has diffused through the film must be equal to the reaction that is taking place on the surface. So we have written that and then the equations what we have written was that minus r A equal to k g C Ag minus C As and if I assume I have first order reaction this is k s C As, okay this also we have written.

So now the global rate of reaction or observed rate of reaction is defined as the rate in which only the measurable variables are present, right. Here the measurable variables is only C Ag and I cannot measure the concentration on the surface which is C As we have to ya why means because here I have to put some (())(2:58) and then try to find out how many moles of oxygen staying on the surface, right.

So that is not that easy and that too it is very very hard surface so any technique which can be used on this surface is normally very very costly technique only for that this Ertl from Berlin University he got noble prize to show how to measure concentration on the surface and he uses the examples like on the platinum surface CO is getting oxidized as CO 2 that example that is one example, another example also ammonia how hydrogen molecules are atleast getting absorbed on the surface and how they are reacting the actual reactions you could show by constructing his own equipment that is why he got the noble prize exactly that is surface phenomena what you could show that is available on his website if you want to go and see that Ertl that is the Noble Laureate name.

So if you go you can also see that it seems during the reaction on the surface there are waves also generated that waves also he has picturized so that is why ofcourse he got noble prize, okay good. So that is why this is very difficult technique to measure on the surface and as I told you as engineers we should see that as simple as possible we should use the technique. So that is why best thing for us is elimination of this and if we eliminate this and then try to write the equation that means I can take these two C As is eliminated so if I eliminate this.

Let me write the other steps also k g C As k s C As, so then I have C As equal to I am jumping the steps equal to ya k g C Ag by k g plus k s, right okay. So now this if I call this one as 1, 2 equation 3 then equation 3 should be substituted in equation 1 because either this or this anyone of the terms.

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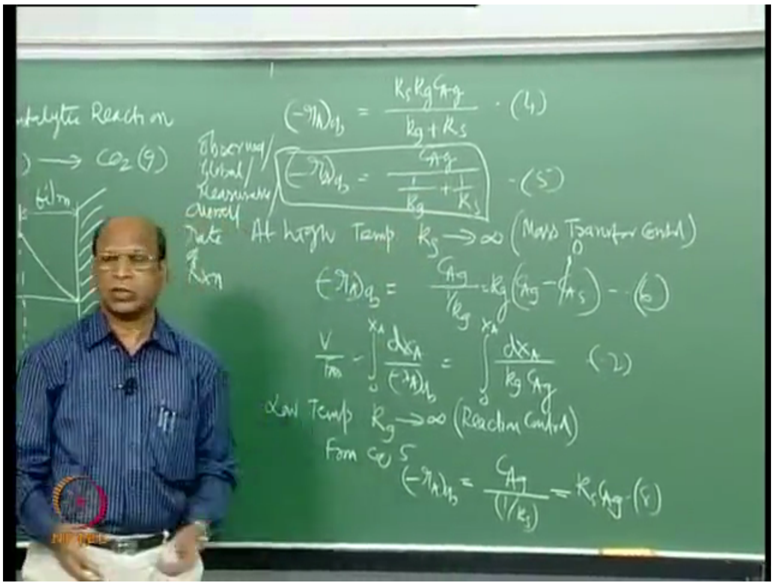

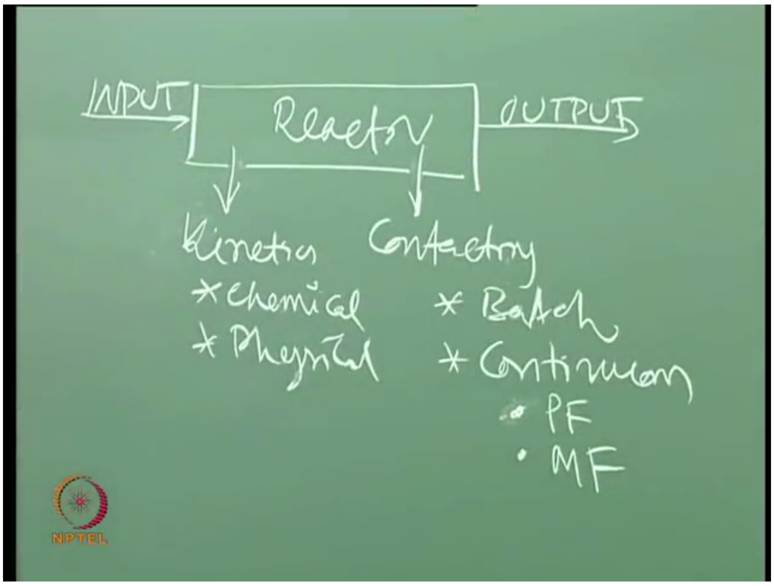

Then I have minus r A ob observed rate equal to if I substitute here in this k s I have k s k g C Ag divided by k g plus k s this also can be written as C Ag divided by 1 by k g plus 1 by k s so this is the rate expression that is the rate expression for coal combustion and this rate expression is peculiar here because we have a mass transfer coefficient k g and also we have a reaction rate constant.

So in general when we are talking about chemical reactions we never take mass transfer coefficient to account but still here in all heterogeneous systems mass transfer coefficients will be automatically coming into picture and if you remember my picture the famous picture which I draw here, this is reactor, input, output, kinetics, contacting, here we have chemical, physical and here we have batch, continuous and in batch again we have PF and MF. So this part we have understood what is batch, what is continuous, in continuous when you choose PF, when you choose MF all that we have discussed.

Now when you come to this there are two terms chemical and physical, chemical is the one which represents k s, physical is one which represents k g. So that is why here you have both now chemical as well as physical that is the meaning of this diagram, right. So that means most of the time I have already told you sometime back that most of the combustion process this is coal combustion most of the combustion processes are mass transfer control ya the reason is that the temperatures are very high so this k s is very very large because Arrhenius equation, okay so when Arrhenius equation you have small change in temperature will be creating large coefficient and now at very very high temperature this is very very large.

So at high temperatures high temperatures k s is large tending to infinity just as an example then we have minus r A ob equal to C Ag by 1 by k g are k g C Ag which we can write as mass transfer equation which is equal to 0 so this is 3, 4, 5 and then 6. Now you see if you assume that for this gas space you have plus flow we have to choose the contacting. So if I I am now thinking that my gas O 2 this is minus A is O 2, right ya so this is moving in the form of plug flow.

So what is the equation we use here for the contacting V by f n not equal to 0 to X A dx A by minus r A minus r A ob. So now I have to substitute this equation that is 0 to X A dx A into k g C Ag this is a reactor design equation but still we have only mass transfer coefficient commutative picture, okay ya so similarly if I have both the controls then I will have this equation C Ag divided by 1 by k g plus 1 by k s that is what is here.

So on the other hand if I have at low temperatures our reaction rate is slow at low temperatures (k s) no k g will go to infinity that means when compared to k s so this here also I will write this is mass transfer control and this is reaction control ya so when k g is very large value from equation 5 from equation 5 minus r A ob equal to we have C Ag this goes to ya this goes to 0 1 by k g and then I have k s 1 by k s which is nothing but k s C Ag so this is equation 7, this is equation 8 ya ya at low temperature the reaction may not be that fast, k s is less reaction is not fast, right at low temperatures, okay.

So that is the reason why k g relatively is faster when compared to k s, right so that is the reason why k g will be very large value so 1 by k g is neglected, then it will be only k s which is the reaction control. I have been giving you this simple example like you know your hostel food, okay I think assuming that you have conveyer belt for breakfast from the kitchen you send the there will be continuously feeding let us say Idlis, okay so Idlis will be put there on the conveyer belt you are there just around the conveyer belt and then as soon sa Idlis come on the conveyer belt if you are very hungry what will happen? You will eat, right.

So practically on the surface what will be the concentration? 0 you will not have anything now which is controlling now? Which is the controlling? Is it the supply of Idlis or is it your eating which is equivalent to reaction here supply mass transfer is control, okay. On the other hand after eating may be every one 50 Idlis you cannot eat anymore, right. So then you will have everywhere concentration that means your rate of reaction rate of eating is almost 0 now very very slow even if you eat because someone is putting a gun and then say that still you have to eat.

So then I know for the sake of eating you may take only piece of Idli and then still you are eating but the rate is very very low that is what is reaction control, it is relative both are relative whenever we talk in this case both are relative. If both are equal then this is the equation which you have to use, okay always in the controlling steps the lowest step will have the control so lowest step, okay.

In these steps these are simple examples which I give so in this step the slowest step controls, here the slowest step means mass transfer because reaction is very very fast and here the slowest step is ya reaction and mass transfer is very very fast and as you said these are all relative, okay good. So now this is the equation what we used and here we are comfortable it is k s C Ag if I take it is like our first order reaction, right.

So we say order of reaction with respect to concentration, in this case it is first order with respect to oxygen if I want to use in the design expression again I go here and substitute this time I will have k s and C Ag and C Ag is measurable that is why we call ya this rate as observed rate observed, or ya another name global, another name measurable very good, is there any other name? Measurable or observed, observed I have given observed, global, measured, overall overall rate of reaction okay so rate of reaction ya.

So all this will come there because when you have heterogeneous system you cannot avoid this observed rate or global rate or measured rate. Why we are telling observed rate is we are able to express this equation 5 in terms of measurable quantities C Ag is measurable and 1 by this k g I should have some correlations anyone of you know what the correlations we used if

I have single particle and then mass transfer is going through this particle or to the surface or inside the surface through the film I have come across that equations single particle we have just only one particle and around the particle oxygen is going and this oxygen is going to the surface of the particle through the film it is external film mass transfer, not able to recall there is one equation called Ranz and Marshal equation it is in the third chapter of table, okay.

And ofcourse Levenspiel non-catalytic reaction also he has given that he call that one Ranz and Marshal but tribal calls that one as Frossling equation Frossling equation, okay.

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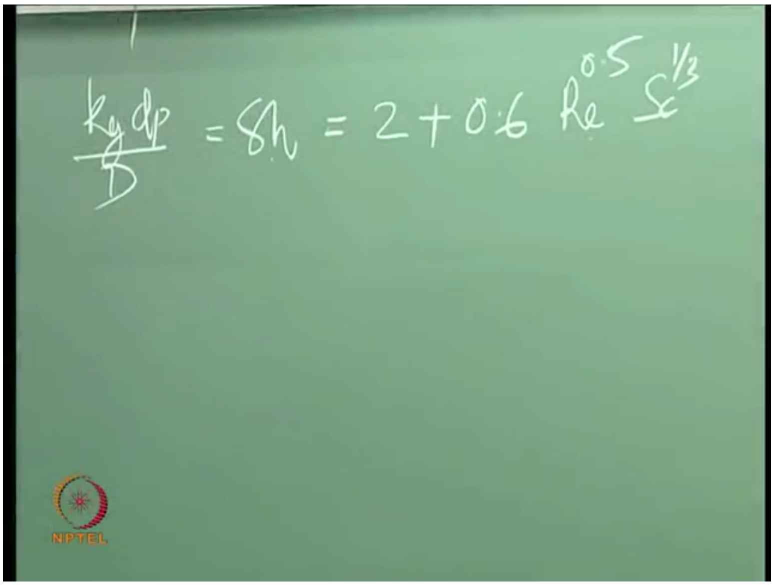

$$\frac{k_g d_p}{D} = Sh = 2 + 0.6\, Re^{0.5}\, Sc^{1/3}$$

So that equation tells us that we will have a Sherwood number equal to 2 plus 0.6 Reynolds to the power of 0.5 and Schmidt to the power of 1 by 3 or 0.33 that is the equation, okay and I think I have to tell you here because most of the time now we will be talking about mass transfer coefficients this is one of the simplest equations in chemical engineering because it is a single particle and in reality you will never have single particle, right and in multi particle systems developing this equation is not that easy mass transfer equations that is why lot of researchers have spent lot of time to develop the correlations even now people are developing if it is a new system.

And surprisingly in chemical engineering if this is for single particle and I cannot use the same thing if I have packed bed the mass transfer through the packed bed is slightly different and I take fluidized bed that is different and all the equations are in terms of only Sherwood number, Schmidt number, Reynolds number you take any equipment like packed bed, fluidized bed, moving bed, rotating drums all these things you know the mass transfer equation contains only Sherwood number equal to the function of Reynolds number or Schmidt number that functionality we have to find out only through experiments, right.

So that is why if you have the same process what we have discussed here if it is in fluidized bed then you have a different mass transfer convention k g I am talking this k g because k g is here in Sherwood number I hope you remember Sherwood number and Schmidt number, Reynolds number you do not remember that is only one number most of the time chemical engineers remember that is why whenever I sit for interviews and all that I ask them other than Reynolds number please tell me other number.

And it is really funny you know particularly there are also numbers in fluid mechanics so other than Reynolds number we cannot list out any other number in fluid mechanics other numbers ofcourse very famous numbers next to Reynolds number is Schmidt number and Prandtl number ya and why all these correlations should have Reynolds number and Schmidt number and here we have even heat transfer coefficient also same exactly same thing.

Here we have now certain number equal to same 2 plus 0.6, Reynolds number will be there and this will be Prandtl number that is the reason why you study transport phenomena because transport phenomena tells you that all these transfers have some kind of similarities, some kind of same phenomena. So that is the reason why in transport phenomena you know you have the famous correlations j d equal to j h equal to f by 2 ya ya why do you need that analogy? We know I mean we know that equation but why do we need for heat transfer ya (())(19:47) also is related f by 2 j d equal to j h equal to f by 2 f is frictional factor by 2 and we need that kind of thing as engineers if I do not have sufficient time to find out mass transfer coefficient I can use friction factor.

But there are many conditions for you know that analogy, right under those conditions I do not have to conduct separate experiments for heat transfer or mass transfer if I know anyone if I know j d I can calculate I can friction factor if I know j d I can calculate heat transfer coefficient, j d is for mass transfer, j h is for heat transfer and f is friction factor that is why that analogy comes automatically for us that is why I told you know chemical engineering is great, the analysis the principles wonderfully demonstrated all the time through equations.

But only thing we do not know is that where they are applicable because I think in 50’s and 60’s that was excellent period for chemical engineering the reason was that a chemical engineering and industry work together beautiful love marriage ya but after sometime in 80’s divorced and the catalyst part divorce is you know what can you guess? Transport phenomena course that is the one because when transport phenomena that book was first published in 1961 or 1962 by Bird Stewart Lightfoot it really changed the thinking of many engineers not only chemical engineers, mechanical engineers use that, civil engineers use that and ya metallurgical engineers use that many people use that I know this transport phenomena.

Then people thought that particular in academic institutions people thought that excellent now any system in engineering now I can model till then it is only imprecision do the experiment develop the correlations that is what because of that only this correlations also has come later these coefficients have been justified by transport phenomena through boundary line theory has come there theory also explained there but it was wonderful in the beginning that imprecision means you have a feeling for what you have done and theoretical highly complicated equations you solve and then finally you find out those coefficients which may not be exactly like you measure and ofcourse any theory should be validated by experiments at the end.

So finally what has happened was many academicians start that they can happily publish and get away without worrying about what is happening in the and when an industry person comes to an academic institution then the industry person was asking some questions and the moment he ask a question the professor always replies in terms of differential equations and differential equations you know industry person has forgot a long time back.

So that is why he thought that my god all the professor started talking a different language it is not industry language. So that is why the distance between those two increased and that is when in some industries they started industrial research that means their idea is to solve immediate to the problems not like academicians, academicians they take a problem and then they have their own phase because they do not worry about industry and time is not money in academic institution. Whereas in industry time is tremendous money one hour gone means may be 1 million dollars also you may lose.

So that was the time when these people have become you have that divorce they are divorced and now ofcourse with Nano technology and all that I think no industry can understand what we are talking so that is also that is greatest contributions what we have these new technologies. So that was the reason why we are not able to get lot of consultancy and all that, particularly in chemical engineering.

But in other engineerings like civil civil still leaves with lot of imprecision they have called I told you know one (())(23:53) called factor of safety their factor of safety may be 5 times, 10 times also, do you know the reason why their factor of safety is high. Our factor of safety may be only 10 percent or you know may be 50 percent, right I think in McCabe-Thiele Method Murphree efficiency normally how much you take you calculate it theoretically 10 plates, right ya divide by 0.8 that means 20 percent you know ya otherwise sometimes 50 percent the reason is that you are not confident about your mathematical analysis because there are many assumptions.

Like that in civil engineering there are many things first of all brick they have to assume some and every person produces brick in a different way. So how can you generalize that they you know the concrete what they make you know they gravel. So theoretically it maybe only often and cheap particle but I think it will vary from 1 nono meter to 1 kilo meter maybe just exaggeratedly ya so then where is the theory coming there on the top of it cement, cement they specify something but you know particularly in we are great in mixing things. So ash will be mixed with cement so then that also gone.

So that is why the factor of safety in a finally building has to leave for some time know or bridge or road whatever so that is the reason why a factor of safety is very very high in civil engineering but whereas factor of safety is minimum in aero spacing they calculate under terms of weight finally for the flight and okay factor of safety equal to 0.5 50 percent okay ya then weight will be 200 tons it will never fly, it will only go at block cart again on the road.

So that is the reason why that factor of safety is less for sophisticated things and electronics also, I do not think electronics they do not have any factor of safety in electronic industry, okay because the problem there advantage there with electronic industry is gravity will never bother them correct no it is only electronics flowing in this way, current will come in this way but where is the gravity coming there? Gravity will never effect.

But in chemical engineering, in civil engineering, mechanical engineering, metallurgy gravity effects and systems are generally very difficult because gravitational force you have to take you know and because of this gravitational force also we talk about again (())(26:21) and all that, right and (())(26:24) we know what is (())(26:25) but we do not know how to really apply for our calculations.

So because of all these problems that factor of safety and all that will come there, okay anyway so that is why this equation is 1 just I have written but I will write many more like that why I wrote equation is from this you calculate what is the equation for Sherwood number? K g dp by capital D which is diffusivity, dp is diameter of the particle and k g is the mass transfer coefficient.

From here you can calculate that k g substitute in equation 7 and then we can integrate because this is the simplest integration then you will get your volume of the system I mean in a simple design I am not saying that all combustions are designed like this but I want to connect that diagram where kinetics and contacting both we can take. So that is the reason why I am trying to tell the simple example they are not real examples in the sense that real examples I will tell you when you come to non-catalytic reactions, okay good so this is how.

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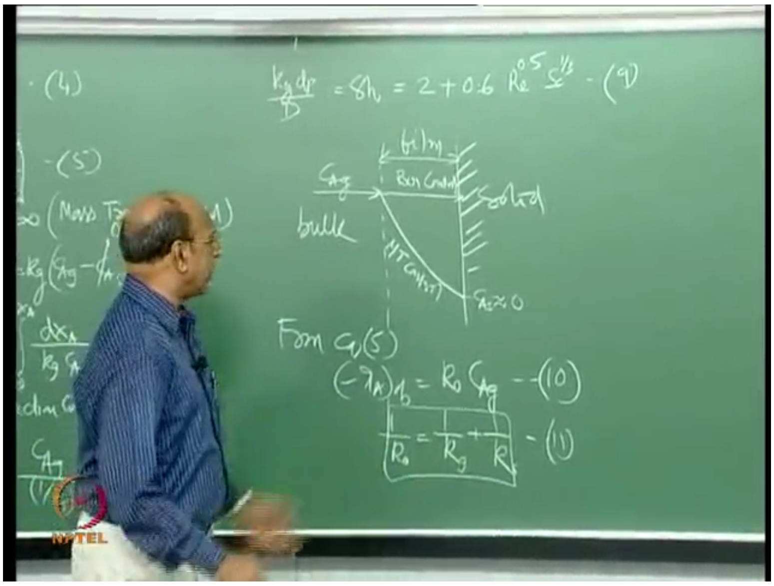

Now let me also tell you here in this profile if I have reaction control maybe I will draw here again the profiles we will redraw this is solid that is carbon, then this is the film and I have here C Ag this is what I know, this is bulk in bulk there is no concentration gradient, okay so there is no resistance for the assumption is there is no resistance for the molecules to go through that film so that is why it is constant, from there if I have reaction control how do I draw that profile?

That means you have to come here if it is reaction control the equation is this one k s C Ag equation 8, how do I draw the profile on the because the profiles are very important in heterogeneous systems. If you draw a clear profiles it is very easy for you to develop the model kinetic model. In fact this is called the kinetic model for gas solid reactions, okay good ya tell me now how do I draw that? Straight line, why straight line? This is correct ya I know just remember the Idli example if your rate of eating is very very less you cannot eat anything, so then entire conveyer belt will have the same concentration of Idlis.

So that is why same everywhere you have the same concentration of C Ag, right okay on the other hand if you have the mass transfer control reaction is very very fast that means you are able to eat very quickly and practically you will see on the surface zero concentration of that Idlis, okay. So you have to draw something like this maybe straight line depends on the geometry.

So here C As is approximately 0 that is why I have drawn here I mean I have written here in equation 6 when you have mass this is mass transfer control, we will write here MT control ya that is MT control and this is what I have given here. You know always for mass transfer you will be very comfortable if you write C Ag minus C As but here C As equal to 0 and for reactor design expression I have to use now mass transfer coefficient there is no more you know reaction rate constant and what are the problems you may face with these?

If you do not know that there is a global rate of reaction, if you know that mass transfer is playing a role in heterogeneous systems and all this we are talking about only at one temperature, okay again heat transfer also comes into picture, okay. So if I take that only for isothermal system I am talking about only mass transfer in heterogeneous systems and you do not know you have these heterogeneous systems.

What do you imagine? You imagine that the rate is proportional to some constant, correct no I mean that is what all chemical reactions the first assumption is minus r A is proportional to C A to the power of n and C B to the power of m, okay and those two coefficients you have to evaluate if n equal to 1 and m equal to 1 then you will have first order with respect to each overall second order all that.

So that is why first assumption is directly proportional to concentrations, right. So that is why even here when you assume the same thing you have from the equation 5 from equation 5 you have minus r A ob equal to k 0 C Ag where k 0 equal to (what is the number) this is 9, this is 10, okay where k 0 equal to or 1 by k 0 equal to 1 by k g plus 1 by k s, right this one I have written as this equal to 1 by k not which will go to the top and then this is k not, okay good anyway.

So this is the equation what you have actually and you think that this is simply k 0 which is some constant but this k not has mass transfer coefficient and reaction rate constant also and suppose I now repeat this is for one temperature what we have done all this. Now I conduct the same experiment with another temperature like another temperature because I would like to find out the Arrhenius relationship.

But now if I and I am imagining that I have only k not which is a reaction rate constant because I have not taken heterogeneous systems, I do not know whether chemical and physical kinetics both will really affect the process, right. So under those conditions I am imagining that I have k not and actually that is a combination of these two, right.

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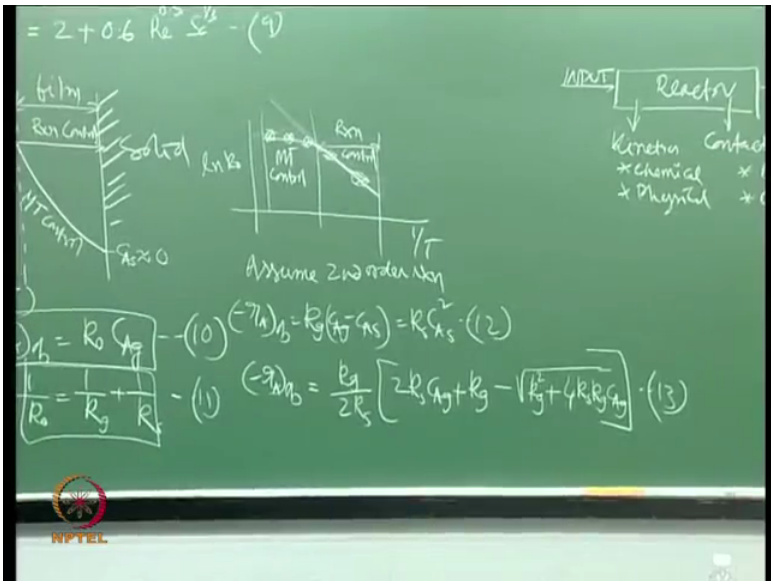

So with temperature if I plot here this Arrhenius plot this is ln k or k not equal to sorry versus T 1 by T then you may get something like this or instead of that I will just plot and then normally how we be we will try to see, okay. So this one like this you may get the points, right because I do not know anything about the presence of chemical and then physical factors affecting the rate of reaction.

Normally what we will try to do we are all experts now going to xl and now choose that option linear because you know it must be straight line. So you will simply draw this which is totally wrong because there is a beautiful phenomena that is coming here, right but on the other hand I will be carefully seeing that why another time repeating the experiments and then finally seeing that there is some problem with this why there is slight curvature?

So if I analyse that I have to plot like this. So that means if I divide this as this zone or also this zone, right. So here it is almost constant within the experiment later, why? Mass transfer and the effect of temperature on mass transfer is not that much, okay it comes as 2 to the power of half 2 to the power of 2 by 3 like that because of the diffusion coefficient, but whereas in this region when I have the reaction control now this goes as exponential.

So that is the reason why if you extend this this will be your normal minus 3 by (())(35:09) line. So you see now wonderful phenomena like MT control here and this is reaction control that means kinetics we are definitely evaluating wrongly if you do not understand the you know the chemical factors and physical factors that are coming into the rate equation that is the lesion what I want to tell you here, that is only point I want to tell you, that means unless you understand the difference between chemical factors, physical factors that are effecting the rate of reaction by simply conducting the experiment and then trying to find out the kinetics and using them blindly may make us lot of error and may give us lot of errors.

This k value this k not which is actually combination of mass transfer coefficient and reaction rate constant, okay if I do not know this then this I am imagining as the first order rate equation ya like (())(36:13) this k 0 I am simply because this is order 1 and here this now I simply take I have the that is equivalent to first order rate constant but actually that first order rate contains two factors, okay.

So that is the lesson which we have to learn that means in heterogeneous systems you have to be careful which is dominating like mass transfer or heat transfer or reaction or all three or all two and here if I have all two this entire equation I have to use, right and most of the time for us likely we have the mass transfer coefficients available in the form of correlations that we do not have to do much work now because any system you take you have some information on that unless you want to design totally (())(37:03) new system, okay and for new system anyway you whole research the whole work you have to do on your own and then confirm that what you have done logically right good.

So now you can see that what I have assumed here is ya here equation 1 it is k s and C As, okay it need not that means here I have taken on the surface the reaction as a first order reaction, the moment I just changed here I have second order reaction everything will change, okay. So why everything changes so the moment I have the second order reaction assume second order reaction then that equation 1 is written as minus r A ob equal to k g C ag minus C As equal to k s C As square.

What is the procedure? What is the procedure we have been discussing to find out the overall rate or global rate or you know other names measured rate ya eliminate C As. Now if I want to eliminate C As this equation number 12 I will write ya 12, if I want to eliminate C As then I have the quadratic equation correct no I have quadratic equation. So I think this I will give as an exercise and if you solve this and then get a first you have to get C As and that C As you can substitute either here or here, okay in any 1.

So if you are able to do that than for second order reaction the rate expression what we get is r A ob equal to k g by 2 k s this is 2 k s C Ag plus k g minus square root of k g square plus 4 k s k g C Ag this is the equation this is equation number 13 this you know how simple equation ya and this is the one which you have to use here again in this design expression ya this here minus r A ob, right so that is what what you have integrate and cubic equation much worse because I think we do not know you may get various forms like negative, positive or you know realistic roots, unrealistic roots, imagine roots all kinds of things.

So that is why you have to really see the effect of physical and the chemical factors on the reactor design I hope now you understood this entire diagram every term has a meaning now for you at this point of time I hope so, okay why because input I know how do you get input? Market survey MBA guys, okay they happily give us so we will take it then kinetics now we have to determine contacting you have to choose choose in the sense that you have to choose whether you have batch reactor or continuous reactor and we have already thumb rules for choosing gas I mean batch system or continuous system Kavya remember when you choose batch, when you choose continuous that is why number of times I repeat do not worry I think you know ya do you remember Rinita?

Student is answering: Reaction times.

No general thumb rules, Anurag you remember when do you choose a batch system, when do you choose a continuous system? I know because you may not remember when I told you that is why number of times I try to repeat ya that is what I am asking when do you need a continuous system? Ya that is general on thumb rule small scale or large scale and you also have another thumb rule particularly for batch systems when you need flexibility in the product.

So today you may produce particularly pharmaceutical one drug, next day another drug, next day another drug like that or pesticides, insecticides and also you have the dice you know suddenly people all people may be interested in red colour if the movie red comes there is some movie called red, okay. So then after words if the movie something about yellow or green comes everyone may be using that.

So this industry has to (())(42:14) to the market for them it is flexible if you have batch systems, whereas continuous system once you design you cannot use it for any other system unless 100 percent overlap of the parameters are there for these two processes process A, process B, right. So that is the reason why once you design continuous system it is dedicated only to that unless otherwise you are very very lucky to have exactly the same parameters, same temperature, same controls then only that is possible, right.

So that already we have that information I know I am repeating this because it is not your interest to remember it is only my interest to remember and that kind of silly thing I may not give you in the examination, okay so that is why you may not remember that is why I repeat many times, okay. So once you have chosen between batch and continuous. In continuous you have again two possibilities, right plug flow and mixed flow.

So when do you choose plug flow and when do you choose mixed flow? Abhinav so you remember or? See all of us want only always higher conversion, okay ya I have given some thumb rules again. Prabhudeva? Excellent, good, why ya gas phase reactions have very small residence times. In fact in the form of only seconds, okay. So and when I have in the form of seconds residence time it is very easy for me to provide residence time in plug flow, plug flow you know that it is definitely more efficient than mixed flow because of the residence time distributions that we have to bring residence time distribution.

Definitely that is efficient that is why all of us would like to happily go only for plug flow but still we do not go many times the reason is if I want to provide 8 hours, 10 hours, 12 hours need residence time in your plug flow reactor I told you the length may be 100 kilo meters, 200 kilo meters because theoretically speaking what is the velocity which will give you plug flow again I am repeating ya Swami, theoretically what is the velocity which gives you plug flow theoretically (())(44:49) okay why infinite and why (())(44:51) tell me there must be some reason know just imagine plug flow, flat velocity profile each and every particle is spending exactly same time.

For each and every particle to spend exactly same time I should have a flat velocity profile, flat velocity profile comes only theoretically if I have infinite velocity otherwise till near the wall you have small droplet small drop there, it is not straight line so that is why, okay. So when I use very very large velocities if not infinite velocities then residence time should be length should be very very large for providing 8 hours, 10 hours length of the reactor and always plug flow reactor the diameters are anywhere you go it will not be more than 8 inches, 8 inches is maximum ya 8 inches is really maximum.

So generally we will go in industries either 4 inches, 5 inches, 6 inches and that is why the reason also there is that you have to maintain that flat velocity profiles to a so that you are very close to plug flow that is the reason why we do all that. So this is the reason why the residence time must be smaller for plug flow reactor. If I have ofcourse liquid phase reaction still the residence time is very very small that means rate of the reaction time is very very small still I can go for plug flow that is again under thumb rule we use we have a plugged flow and mixed flow whenever we say that we have gas phase reactions where we have very small residence times required for this reaction to take place then you go for plug flow.

And very large residence time mixed flow is easy for me because it is a tank. So any amount of residence time I can really give if I have a tank reactor because only length by diameter l by d will just increase that is how I told you three weeks is the mean residence time for wastewater treatment plant and did you see any time wastewater treatment plant, no never Rinita who has seen wastewater treatment plant you have seen?

Ya what is the size when you saw that big ponds ya if it is normal water we can even swim there all of us can swim not only one, okay. So it is not you know tub bath or something you can really go one or two (())(47:24) this side that side really that big that big is very easy for me because three weeks residence time easily I can give them so that is why that is why in industry for large productions even tank reactors will be 1 meter cubic 1 is not smaller 1 meter cubic is very very large 1000 litres okay or 2000 litres you have to put the size.

So that is the reason why tank reactors I can provide any kind of residence time that is one thumb rule, the second thumb also I told you temperature control highly exothermic reactions even if it is gas space but very very sensitive okay that means one temperature 1 degree that is why this way we may catch fire, okay. So I mean that (())(48:11) definitely we have to avoid otherwise you know you will not be there or the persons working in the industry will not be there totally because explosions, right.

So that is why under those conditions we can again go for a mixed system, one of the beautiful examples are you know Phthalic Anhydride I think to produce nylon or something, it is a catalytic reaction but highly temperature sensitive it is a catalytic reaction. So first they tried packed beds but when they tried packed beds it is very difficult in the sense that temperature control they are really worried every time when they go to the plant for operation the operators must go to 10 temples atleast and then pray the god and then go to the industry otherwise there is no guarantee that they will come back safely even then there is no guarantee but it is only okay but only for our safe our (())(49:03) will go there and then pay and then come back, okay.

So that is why there they have gone to fluidized bed where fluidizer system give some kind of mixing temperature control is beautiful there, in fact it is the same story what I have told you is also given in Levenspiel gas solid systems catalytic reactions, okay so that is why. So now we know that when do you choose that batch system and when do you choose continuous system and ofcourse when do you choose plug flow and when do you choose mixed flow please do not forget this, okay please do not forget I think you know number of times I can repeat I will be repeating but next time when I ask you please answer that, right.

But I think by repeating ofcourse I do not blame you that is why I am repeating most of the times and atleast this diagram we should thoroughly understand I said, all other things are details calculation of volume if I am using mixed flow or plug flow or batch reactor that is the detail later. But right now the concept of that what are the things that are involved in the diagram, right I hope input we know, contacting when do you choose between batch and continuous and in continuous again when do you choose mixed flow and plugged flow that we know.

And this one is kinetics next one kinetics chemical and physical kinetics the meaning is chemical and physical kinetics meaning is the steps that are involved the steps that are involved. Here I have actually that is why in the last class I have given those three steps and all that is what I have not written here. So in the last class we have written there mass transfer from bulk to the surface, then the rate of reaction, then diffusion of oxygen sorry CO 2 back.

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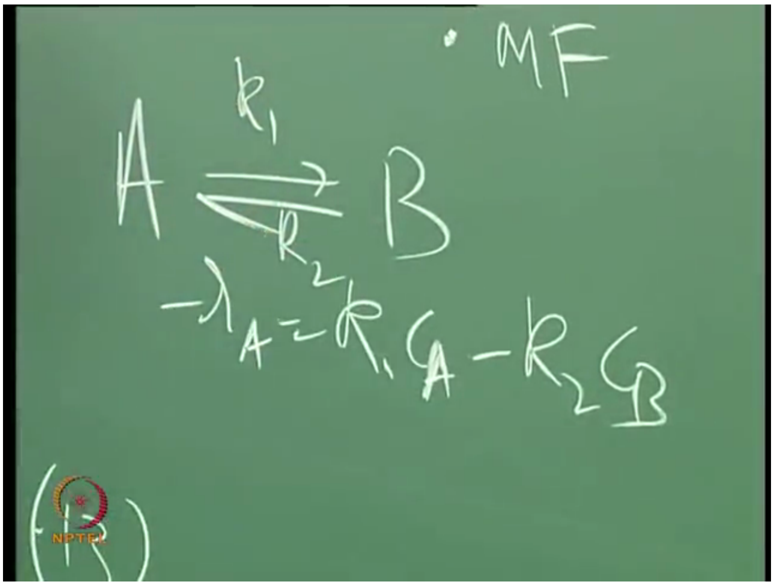

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$$A \underset{k_2}{\overset{k_1}{\rightleftharpoons}} B$$

$$-r_A = k_1 C_A - k_2 C_B$$

But because it is irreversible reaction oxygen coming through the film will not affect my rate of reaction, if it is reversible reaction the reversible reaction depends on again you know the ya product concentration also A going to B. So I know here it is minus r A equal to k 1 so that it can remain k 2 C B right reversible reaction this is k 1 and k 2 ya so if I have a reversible reaction the product also affects C B is the product B is the product.

So but here in this example I have CO 2 coming but CO 2 is not participating in the reaction that is the reason why I have to take only two steps mass transfer to the surface, rate of reaction on the surface and under steady state conditions both must be same and those two we have written here this is the procedure for all heterogeneous systems I have given one but I think in the tomorrow’s class I will also just draw the profiles for another two, three systems so that we are familiar with simple drawing you know profiles.

And this imagination is a must I tell you please open up your mind and then have this imagination like I told you here how the carbon is burning you take one particle and there is a flame and anyway fluid mechanics will tell me that there is a film which you cannot see around this but oxygen has to diffuse because oxygen is not available on the surface it is available only in the bulk it has to go through the film and then reach the surface.

Then on the surface you should have sufficient temperatures and conditions for reactions then rate of reaction takes place, then the product gases will come out if there is no product gas no problem that is fine, okay and so many steps are involved out of that what are my important steps and how do I show them as pictures all this is imagination what I have done and now this is the picture and this picture leads to me just draw the profile ground right this is the profiles.

Like that I may have some three, four steps and everywhere I have to draw the profiles and list out what is step 1, step 2, step 3, step 4 and you will see here most of the time reaction is only 1 step and mass transfer steps can be 4 or 5 that is why mass transfer is so important in heterogeneous systems particularly if you take our dalda reactor salary reactor there are 4, 5 steps involved and you take normal catalytic reaction simple catalytic reaction if I have this is the particle and similarly the reactant is going that A going to B and it is not reversible reaction we assume that it is a reversible reaction, catalytic particle A is going around so now this A has to diffuse through the film first because the reaction is taking place only inside the particle because this is porous particle here atleast we have assume it is not porous particle, right.

So I have the particle and then going around this and you have now first step is mass transfer through the film, second step is it is porous particle, mass transfer is through the pores and when it is going through the pores it will also get adsorbed and if I look at one molecule this one molecule has to go from bulk to surface through the film step 1, step 2 it has to diffuse through the pores and after diffusing some distance it has to get adsorbed, after adsorption it will form a complex and all that people say and then after words it will get dissociate and then product is formed that is reaction, adsorption and then reaction.

After reaction the product which is formed there has to dissolve dissolve so that is fine and after dissolving it has to come out through the pore that is 6 and then it has to again come out through the film through the bulk 7 steps which one is controlling we do not know that is why in heterogeneous systems a kinetics is really hell that is why happily we ask chemist to do that, okay you develop Langmuir-Hinshelwood kinetics you know Langmuir-Hinshelwood kinetics you know all these 7 steps and we are also going to derive some of them and I will also show you at the end one all 7 controlling what kind of equation you get all 7 steps controlling.

And unfortunately in all this is that you have these constants you know k g, k s in this catalytic reaction you have two mass transfer coefficients steps, okay and then adsorption, desorption all these constants, surface reaction all these constants are involved there. So you have to determine from the experimental data these constants very very accurately that is why chemical engineers are also should be very good you know mathematicians I am not saying mathematicians to develop new theorems and all that but atleast for using the mathematics that are available atleast with us so in the in analysing our data.

And you know how difficult it is to evaluate this constant k 1, k 2, k 3, k 4 more than two we have always difficulty in evaluating the constant I am telling. So how do you find out normally I have the rate equation, I have the experimental data now rate equation has k 1, k 2, k 3 now I have to fit this entire data to give this k 1, k 2, k 3, right. Matlab is one which will help us, right and then the Matlab we will go at them we will use some values and it evaluates k 1, k 2, k 3 and then give 0 you bring those constants.

Then I also done the same experiment and same data in fact I also want to analyse using this k 1, k 2, k 3 to evaluate then I will give you a different gas value then my values and your values may not be unique that is a physical system it must have only one unique set of values this is what is the biggest problem if I have more than two parameters that is why Levenspiel beautifully tells that you may produce any number of wonderful models for publications but for industry you should give atleast the minimum you know one is the best one or two two parameters models.

He never complicates things because the moment you go more and more 4, 5, 6 and all that I do not have any physical meaning for that no physical meaning for these values, okay I think I have already told you sometime back maybe residence time distribution I do not know Anurag did you do CSTR with dead space and by pass a model for CSTR or mixed flow with dead space and by pass you have not do it, okay.

There you will have three parameters which is called a bypass fraction, a dead space fraction and dead space is not really dead definitely there will be you know mixing some kind of exchange between dead space and at two zone what we call exchange coefficient all these three. Bypass has a definite meaning 20 percent bypass, 30 percent bypass, okay and what is the other one dead space has a definite meaning maybe 10 percent dead space or 20 percent dead space, 100 percent cannot be dead space, okay that is very bad design, okay ya.

So then this exchange coefficient depends on what kind of mixing is going on three parameters. So if I evaluate data if I get a set and if you evaluate if you are getting a different set what is the physical meaning for this? I may be telling that I have 15 percent dead space, you may come up with 30 percent dead space but that system at that particular conditions it must have only one set of values that is why that uniqueness in evaluating these constants is one of the biggest challenges (())(59:01) even if you do research at (())(59:04) when you have more and more I do not know how really I will appreciate this by a technology people where they will have 25 parameters.

And mechanical engineers for combustion 400 parameters for combustion, okay. Really if you see that there are so many models with lot of constants I use to wonder how are you going to evaluate all these 400 parameters 400 constants. So that is why as engineers we should present our system, experimental data, modelling should be as simple as possible, beautifully Einstein told that model can be as simple as possible but not simpler this is a wonderful statement what he has made you can make your model as simple as possible but not simpler.

So that we have to remember and then I think I will give you some examples in the next class and after the next class then we will go to non-catalytic reactions first, I think I have not told you how do I evaluate you till now because I thought I will give you this introduction for that particular figure and then tell you that.