## Chemical Reaction Engineering 2 (Heterogeneous Reactors) Prof. K. Krishnaiah Department of Chemical Engineering Indian Institute of Technology Madras Lecture No 11 Designs of Non-Catalytic gas solid reactor Contd.

Okay yesterday we have been discussing about design of a non-catalytic gas solid reactors and we again went to my diagram that is kinetics contacting input output and all that, so then we have also discussed what kind of contacting pattern you will get, right depending on the type of reactor you are taking that means it is a blast furnace, rotary kiln, fluidized bed, moving bed all various reactors what you have for non-catalytic reactions and the precursor for that was that we should know the kinetics first and I hope you know the kinetics till now what you are talking about is non-catalytic gas solid reaction kinetics okay. To summarise I will give the equations which have to be used for the design.

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So the kinetic expressions what we have kinetic equation for a gas solid non-catalytic I will write again NC non-catalytic reactions. So you know if it is only film control anyway for 3 control you have the big equation and that has to be (())(1:34) at the end but individually if I write if I have film control what you have is equation t equal to rho B R, 3bkg C ag X B. This is the one which I asked you to re-write, so tau is rho B R, 3bkg C ag we know this equation comes when X B equal to 1 and t by tau is X B this is very nice simplest equation t by tau good.

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So now if I have diffusion control ash diffusion control number 2 you should remember this otherwise in the examination you will have the problem okay so t all over individual steps rho B R square, 6b C ag De so this is only slightly complicated 3 1 minus X B to the power of 2 by 3, 2 into 1 minus X B this is equation, this equation is 4 and tau is rho B R square, 6b C ag De so this is equation number 5. Then t by tau equal to 1 3 X B to the power 2 by 3, 2 into 1 minus X B so this is equation, so this is equation number 6 there is a meaning why I am writing all this okay. Then you have 3 reaction control, so here t equal to rho B R, b C ag k s into 1 minus X B to the power of 1 by 3 this is 7. Tau equal to rho B R, b C ag k s this is equation number 8.

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Now t by tau for reaction control is 1 1 minus X B to the power of 1 by 3 this is equation number 9 and all this is for constant size particle right okay. Constant size particle of course here you can also list out there just leave a space and then you can list out all 3 controlling that equation also you can just leave it there I am not writing that and now if you have changing size, if I say that this one has A.

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B. Changing Size particle  
(1) Film Control  

$$t = \frac{I_B R}{b k_0 G q} \left[ \frac{1 - (1 - \chi_B)^3}{n + 1} - (10) \right]$$

$$T = \frac{I_B R}{b k_0 G q} \left[ \frac{1 - (1 - \chi_B)^3}{n + 1} - (11) \right]$$

$$T = \frac{I_B R}{b k_0 G q} \left[ \frac{1 - (1 - \chi_B)^3}{n + 1} - (11) \right]$$

$$T = \frac{I_B R}{p} \left[ \frac{1 - (1 - \chi_B)^3}{1 - (1 - \chi_B)^3} - (12) \right]$$

B changing size particle that means during the reaction size of the particle continuously changes and here we have for film control you have t equal to rho B R b k g naught C ag into 1 minus 1 minus X B to the power of n plus 1 by 3 divided by n plus 1, this is equation number 10, so tau is rho B R, b k g naught C ag n plus 1 this is equation number 11 then t by tau equal to 1 minus 1 minus X B to the power of n plus 1 by 3 correct this is 12. I hope you know the value of n or small particles, large particles n varies from half to 1 okay depending on the (())(7:33) small particle and a large particle and next one is reaction control.

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For reaction control t by tau is given by equation yes equation 9 t by tau okay, for reaction control t by tau is equation 9 (())(8:06) repeat again. So these are the equations you should remember for the design because this is the kinetic models right so which will give you the relationship between X B and t by tau or t because tau also you know good. So once I have this then the next one is contacting right contacting and yesterday we have discussed about contacting saying that whether you have blast furnace if you flow through that for both the face are plug flow.

If you have rotary kiln again both faces move in plug flow and if you have fluidised bed then solid may move in mixed flow and gas may move slightly difficult to find out and when we are doing fluidisation, fluidised bed reactors then you will know exactly what kind of pattern you will have that I will tell you later but to start with if you want to assume you can assume when you are near minimum fluidisation velocity it will be almost plug flow right. I mean there are people who can assume even mixed flow for a gas also but that must be at a very high velocity somewhere as you know in fluidisation is the minimum velocity that is required for fluidising the particles to keeping the particles in suspension night and there are very high gas velocities where almost terminal velocity are reached.

So if you reach terminal velocity it is no more a fluidised bed is a transport bed you know all the particles will go out okay. So that (())(9:37) and all those things we will discuss that later and if you have a moving bed, moving bed means you take a cylindrical tube may be 1 foot diameter and hide maybe 20 feet, 30 feet, 40 feet and you may send for example your iron ore slowly from the top right and from the bottom you may send your hydrogen or CO so then

this will react, gas will react the solid and we should have sufficient conditions for the reaction to take place then what kind of contracting pattern you can take for moving bed, both are plug flow okay because in the moving bed you are allowing such that you are full of the entire column as a packet bed and then just remove the some small hole you know with a control of the valve.

So that fixes the actual flow rate from the top and bottom. Then the entire bed will be slowly moving down that is why we call it moving bed reactor, so that is why any reactor you take we can always break into our basic contract in patterns whether mixed flow or plug flow, so once we do that then we should also think one more thing we should also take one more thing in to account this I have mentioned in the beginning as usual I think you may not remember I told you that our most important phase is solid in non-catalytic reactions in many cases okay almost 99 percent of the time we are more worried about what is the conversion of the solid rather than what is the conversion in the gas phase, so that is the reason why solids are our important phase and once you have solid as important phase then we have to treat the solid as what is called macro fluid.

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I do not know whether you have...okay I will write here macro fluid okay and that is why the knowledge in reactor theory is also important here you have forgotten what is macro fluid and how do you get an equation or macro fluid all that then it may be slightly difficult or you but I will just try to give the brief election there okay good and I have also given you the formula sheet for reactor design you know some time back in the class earlier, so there also for macro fluid what is the equation and how did you derive that? That is very important here,

so conceptually what we are thinking is that in one of the problems with RTD is that it cannot solve or it cannot give complete information to calculate conversions and RTD can gave the information only for first order reactions, why?

Because first order reactions conversion depends on the time and RTD gives you that kind of information so direct combination there. So RTD gives me the time, what is the definition of RTD? You know the time taken you know the fraction of material which is coming between time t and t plus Delta t, so if I look at my reactor and if I want to find out what is the fraction of material that is coming between 10<sup>th</sup> minute and 11<sup>th</sup> minute right so that fraction is E t dt where ET is the existed distribution function and DT is the time interval that is the fraction, so now if I can add all those fractions then I will know that the total amount of material how much time it took then I can take the average of that then I will take the mean residence time or average residence time all that you can get from RTD but if I take other than 1<sup>st</sup> orders in 2<sup>nd</sup> order okay is one more parameter which comes into picture that is called mixing whether the mixing has taken place early or mixing has taken place late and one of the beautiful examples that was given for this to demonstrate is this.

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I have a plug flow reactor then followed by mixed flow reactor and just reverse the same thing yes these are the 2 models right, so this is ideal plug flow ideal plug flow, ideal mixed flow ideal mixed flow right, so I have this 2 systems and if I conduct a 1<sup>st</sup> order reaction whether here or here I get the same conversion right and if I conduct the 2<sup>nd</sup> order reaction this will give me more conversion and this will give me less conversion, so the idea here is

that here in the  $2^{nd}$  order reaction we have to keep the concentration as high as possible because we have KCA square as the rate.

So if CA is large then you will have more and more rate of reaction and then more conversion correspondingly okay so that is what is happening that means you should not allow mixing for higher order reactions greater than 1 okay you should not allow in the beginning itself so that means you should delay the mixing as much as possible. Here it is delayed 1<sup>st</sup> I have plug flow where by definition there is no mixing we are talking about action mixing okay good. So whereas here if I conduct the same 2<sup>nd</sup> order reaction it gives me low conversion because here at the 1<sup>st</sup> instance itself you have the concentration decreased because of perfect mixing.

The idea here is when fresh concentration CA naught is just put inside then this will mix with... Already there is a continuous flow, continuously reaction is taking place, so this fresh CNR is mixed with already converted stream within the reactor where the concentration falls right. Product has a different concentration in the outlet or here it is same concentration, so that is why it now gives low conversion here and (())(15:53) other and less than 1 this will give you more conversion and this will give you less conversion it can be proved and you can derive on your own it is not great e equal to MC square type concepts here it is very simple, so that is why you can...they are on their own and then try to find out, so that is why now the question came here that okay you are telling about this is late mixing and this is early mixing okay this is late mixing and this is early mixing.

Can you say how late it is or how early it is because early and late are only you know relative terms I thing they are loose terms. General English only will use that but you have to be very precise in engineering to say that late means how many days late how many hours late. So that is why we cannot that that kind of information in these 2 systems right, so that is why we imagine a fluid where if I have broken up all my fluids which is continuously going inside in terms of packets where these packets are not allowed to coalesce or allow to break. I hope you know what is meaning coalitions and breaking of course you know okay.

So we should not allow that means once the packet enters as a packet it comes just like that outside okay this we call it as segregated fluid okay or we can also call this one as macro fluid and the other extreme is the Micro fluid where we have individual molecules freely moving throughout the reactor, so that means any molecule if there is a chance for reaction, any molecule can react with any molecule because there is perfect mixing. In this perfect mixing is possible in micro-fluid you should not get confused here but even this micro-fluid there are 2 restrictions the status of the fluid itself, the fluid can easily move in the form of individual molecule that means there is a possibility for the molecules to interact with any molecule in micro-fluid right but that is one restriction, the other restriction is that suppose I put that in a plug flow reactor these individual molecules micro-fluid now I put in plug flow reactor but by definition plug flow reactor is not mixed reactor you are not allowing molecules are capable of moving but your system will not allow the molecules to move that is why even micro-fluid behaves as macro fluid there okay.

So in a plug flow whether I have micro-fluid whether I have yes macro fluid or micro-fluid it does not matter for me because the treatment is same. What we see is every particle is entering and exactly leaving at the outlet with the same time whether it is packets or whether they are individual molecules, so the residence time is fixed for the packets that is macro fluid or for the individual molecules and the reaction is taking place when it is slowly moving and that is why we say that we have in finite concentration across the cross-section okay I mean not infinite cross-section it is infinite mixing, so that means infinite mixing idea is here at any cross-section if I look my concentration is same but that concentration is varying with axial direction okay, so now good. So as far as this individual molecules are concern we have understood now okay in the individual molecules are able to put in mixed flow reactor they are capable of easily mixing, so actually it will get diluted so that is why you get also less conversions.

Now how do I put this same information with macro fluid I will now take these packets of molecules and then pack here and then okay continuously I feed and then they come out. Now even the packets the concentration is uniform because if I look all the packets will be exactly moving like this okay, so then I can find out all the concentration here is same, concentration here is same, concentration here is same okay within that line, so again it is easy for me to imagine for plug flow but if I put do the same packets here in the mixed flow reactor then by definition the residence time distribution that means molecules coming from the start to end it is 0 to infinity that means some molecules may stay almost 0 times and some molecules may stay infinite time that is molecules wise.

Even if you take packets some packets may stay 0 time some packets may stay infinite time and each packet now you can imagine as a small batch reactors. They are not allowed to mix with any other packet right, so that is why the reaction that is going on is only limited to that packet that packet alone right. So now the concentration or conversion that packets depends on how much time it has spent inside the reactor, so some may spend only 5 minutes some may spend 50 minutes some may spend only 5 seconds, so in 5 seconds packet the conversion is almost 0 or let us a very small and 5 minutes you will have some corresponding conversion or 50 minutes almost the conversion would have been completed okay conversion should have been one.

So that is the reason why the average of all that that is the one which you see outside and I can also tell you like a story like the story only I am now trying to tell you, so now we can tell that if I have a macro fluid okay and if I have 2<sup>nd</sup> order reaction, 2<sup>nd</sup> order reaction, macro fluid, mixed flow reactor remember 3 conditions mixed flow reactor, 2<sup>nd</sup> order reaction, macro fluid and the other case is again okay mixed flow reactor now micro-fluid not macro fluid, micro-fluid and 2<sup>nd</sup> order reaction which one will give you more conversion? You were telling something.

Student: (())(22:27)

Prof: Why?

Student: Because (())(22:32)

Prof: Yes, so what is happening? Correct the answers right.

Student: Concentration is retained by that packet.

Prof: Excellent concentration is retained by that packet as high as possible, so that is why you will get more conversion when compared to micro-fluid right okay I think this is the general information I think this has to be...you have to remember all these things it is a wonderful concept and remember this which will make everything clear okay, so that means if you put 1<sup>st</sup> P of R and then M of R and reverse it and you will see that here you have more conversion per second order year you will have less conversion per second order and then the reason you have to question why? Why that is happening?

That is happening because that is late mixing this is early mixing for a 2<sup>nd</sup> order reaction, so then everything falls because I cannot define even now we do not have complete picture in react engineering how to get that information we are asking that means you know one extreme only you are discussing at means you are allowing only packets in one case and all individual molecules in other case but in reality you may have some packets and some molecules individually then under those conditions how do you do that? Many people tried

wonderfully and there are very nice models and all that but still we are not perfect and trying to get the conversion (())(23:56) reactor okay. Now what is the connection between this this what I told and also now the design in non-catalytic reactors right. I told you that are important phase in most of the time non-catalytic reaction is solids. Would you take solids as micro-fluid or macro fluid?

Yes if I take iron ore particle of let us say may be 1 centimetre then inside that you have so many molecules of a Fe3O4 right so that one is like that you can imagine all the particles are as macro fluids right, so once you have that macro fluid now how do you find out the conversion for this macro fluid? Even here if I have this I told you that imagine that only we have mixed flow reactor the other one also we can imagine at this will give you slightly more information then continuously I am putting the packets and continuously they are coming out on a steady state condition but when I am concentrating at times t equals to 0 let us say 100 particles 100 macro fluid packets I just put it there then out of that one may come out right immediately then afterwards may be 5 minutes, 10 minutes all that you may come out.

Now what you trying to do at the end you have to average the concentrations of all these packets within that batch what you focused, so like that continuously any time you imagine that is what is happening continuously I am feeding the packets, continuously they are coming out but depending on their own residence time you will have conversions and all that average conversion is what I see at the outlet okay, so imagination here is that all those packets have been broken into molecules and then try to find out what is the conversion there, so then there that is what we see but actually what is happening is each individual packet will have a different conversion you are averaging all that, so that means what is that mechanism? What is happening there? I have let us say between may be 5 minutes to 5<sup>th</sup> minute to 6<sup>th</sup> minute how many packets have come what is a conversion in that okay.

How do I get the information on 5<sup>th</sup> minute and 6<sup>th</sup> minute? How do I know how many packets are coming? Do you have information or you do not have information. Question is clear I am just asking I want to find out in any reactor mixed flow we are talking, so what is the...what number of packets come in between 5<sup>th</sup> minute and 6<sup>th</sup> minute, do you have that information? RTD instead of packets instead of fractions I said packets that is all, so RTD will give you between any 2 times what is the fraction of material that is coming out and now the kinetics if you have 1<sup>st</sup> order or 2<sup>nd</sup> order that the kinetics will tell you now what is the conversion in those packets, right?

So between 5<sup>th</sup> minute and 6<sup>th</sup> minute I have 100 packets or the fraction maybe 10 percent of the material okay, so within that what is the conversion and that conversion is dictated by kinetics, so that is why kinetics and contacting this RTD is nothing but contacting right and if I take ideal mixed flow reactor I have a specific RTD right because mixed flow I am telling, so when I have mixed flow specific reactor then I know definitely my RTD the reverse is not possible there is also a wonderful point which we have discussed last time, so that means given a reactor you know definitely what is the RTD okay.

Here if I give you I have a mixed flow reactor then you know the equation is yes ET equal to E4 minus t by t bar by t bar that is the equation what we have right but if I give you this equation and then ask you what is the contacting pattern you can generate infinity, infinite number of possibilities are there this is again a wonderful point I think you have to remember okay we have discussed that in the last semester. So you understood the question? I think it is very nice given a reactor you know definitely what is RTD but given a RTD function, RTD equation you can never say what kind of reactor you have but only one condition is that if you have plug flow direct delta function no other system can give you direct delta function.

Direct delta function is the RTD for plug flow, no other system can give you that direct delta function except plug flow but whereas with mixed flow there are many possibilities. There is nothing new or totally weird thing what we are discussing because it is already been discussed by (())(29:05) for long time in his book okay all other books also right but (()) (29:10) gives that beautifully so that is why I thing you have to read once more all this information. So that is why when you go for actual writing the equations then we need this kinetics because this is what which gives me what is the conversion that is going on in each and every packet this one all these equations depending upon film control, depending on ash diffusion controlled or reaction control depending on 3 controlling that is also... Right that will give me in those packets like what is the conversion and my E t dt will give me what kind of reactor we have okay, so based on that only we have derived that equation for segregated fluid okay.

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Design expression for macro fluid okay here we have the macro fluid for solids, yes we have 1 minus X bar B equal to 0 to infinity 1 minus X B of single particle into E t dt, so this is equation 13 so this is the equation. I have written this in a slightly different form than what I have given in the formula sheet okay, so actually what is this one here Ca bar by C naught and this is Ca by Ca naught batch okay here it is single particle. Now you can see if I have this E t dt for plug flow reactor so then this becomes direct delta function.

If I have mixed flow ideal reactor so then again you have here E4 minus t by t bar by t bar, so those things you have to just substitute there and it is not only ideal reactors, any non-ideal reactor also this is true. Yesterday Sachin was asking me in blast furnace where if you do not have ideal plug flow what you do? If I do not have ideal plug flow what is the nearest non-ideality that comes for plug flow axial dispersion. We have an equation for E t dt or ET for axial dispersion that is what you substitute here. If I do not have ideal mixed flow reactor then we have a mixed flow reactor that space because mixing is not perfect and that happens many times in fluidised bed also because some part of the bed is not that vigorously mixing that vigorously fluidising and some other part in the bed because in industry you will have 3 metres, 4 metres diameter fluidised bed okay 4 meter I think it will be three fourth of this room that is the diameter what you have.

So some part it may be very active some part it may not be active because of non-uniform distribution of gas, so that is why you have (())(32:44) spaces there, so you also have a model for ET if I have (())(32:49) space and by pass okay. So that is why you have all the information and also gave you last semester that you have so many models also, possible

combination of models for E t dt you know for residence time distribution model I also gave a hand-out there at that time, so that is why all that information can be used in this equation right okay, so normally what happens here is that when I put 0 to infinity as the upper limit is it really realistic or do you want to change that value physically. What do you mean by infinite time? What will be X B 4 infinite time? Yes so that entire integration disappears so then what is the logical upper boundary?

Student: Tau.

Prof: Excellent tau. Tau is the logical upper boundary.

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So this equation is one minus X bar B this you write 1<sup>st</sup> then this is 0 to tau, see beyond Tau you do not have X P equal to 1 so that functions disappears okay, so that is why you have to put only this maximum is tau this is single particle E t dt this is the actual equation yes and of course and now if I have this ET for ideal plug flow or ideal mixed flow now I can substitute and then get the values okay this is the general expression for yes I think I will actually write maybe tomorrow all these things the actual equations we write for plug flow as well as mixed flow reactor and what I would like to tell is here this X B is not an easy function except for this.

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This X B is simply one minus I can add 1 minus, 1 minus X B okay so this equation yes I do not know whether you have realised that or not E t dt is in terms of time and X B also have to convert in terms of time so that is the relationship what I have been telling you know you need the conversion time relationship from kinetic models, so that is why this equation gives me that relationship 1 minus X B now in terms of t time, tau is constant anyway and those things I know how to calculate, so that equation you have to substitute here if it is film control here I have to substitute 1 minus T by tau here and then here I know if it is a packed plug flow or it is ideal mixed flow then I can integrate that equation. Integration is not easy I think normally a complicated equation only you get okay.

Now you see diffusion ash diffusion controlled yes so this is equation which I have to solve first I have to get from this equation 4 1 minus X B that 1 minus X B should be expressed in terms of t or t by tau okay this equation, equation 6 this is easy instead of writing all that things.

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So T by tau so this X B or 1 minus X B has to be solved and then substitute there and integrate, so you know this is a cubic equation now and then it is not that easy and even here the other one yes this is easier than this okay, so that is why I have written all these equation in this fashion so that you will have immediate relationship between this design expression and then that this is the final (())(37:05) expression, what you get from this? If I give you time maybe you know we have in terms of time here right, if time is let us say 20 minutes, 30 minutes, 40 minutes what is the conversion? Okay or of course if you substitute after integration these limits that will be in terms of t by t bar t bar by tau. Tau is associated with individual particles please remember that tau is associated with individual particles, t bar is associated with reactor.

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Yes I thing may be you did not catch my point here if E t if I write as E power minus e by t bar by t bar this is let me say clearly M, so this they will disappear because it is a definite integral okay this t small t then you will have in terms of t bar M and tau yes minus is there okay so that is what so you will have the equation only in terms of t bar and tau, tau we know anyway okay that is no problem. Now given X bar B calculate t bar, t bar is associated with again I am telling you the average residence time of the particle. How to calculate? Volume by volumetric flow rate right but in this case it is not volume by volumetric flow rate.



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It is hold up by w is hold up kg by F what we call kg per time, so t bar I know now okay so we have to find out this t bar if x bar is known. If t bar is given to you I will say that okay I

have so much you know the hold-up inside the reactor and I know what is F the flow rate that is actually your input (())(39:24) your input here okay, so then I can calculate t bar using that t bar I can now calculate what will be the x bar. It is the same thing, same design if you know the volume calculate conversion, if you know conversion calculate volume you cannot do anything if you do not know either this or that okay at least one you should assume one you should know okay so I think we will stop here.