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Lecture - 30 Design of Chemical Reactors (Contd.)

Hello and welcome back. We have been talking about the generation of multiple steady states or the so called multiplicity of steady states in CSTR. So, the topic of today's lecture is remains the same as the previous one that is the design of chemical reactors. So, we go back straight to where we left in the previous class.

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So, we have been discussing this particular graph here and with relation in relation to you know, if you remember this equation energy balance equation, the left hand side is a rate of heat generation, right hand side is the rate of heat removal and both are equal at steady state and of course, this equal in these particular equation because we had derived this as a steady states situation for CSTR and as we told if we plot this side as a function of temperature then temperature of the reactor then we have this rate curve.

This is the rate of heat generation and if we are plotting this side as a function of reactor temperature, then we have this curve and we can have several these curves depending on how we vary this T prime that is and corresponding to that you can operate as a particular condition at which these 2 curves intersect only once, then you are operating at that one steady state, you have available for the reaction or they can also cross twice or thrice, when it is thrice, you have 3 steady states available and then we discuss these things in little bit more detail and we told what does this mean to be having 3 steady states in your at your disposal. So, this steady state means the corresponding temperature. So, the reactor you know. So, you can operate the reactor at that particular temperature and correspondingly you have this line.

So, with respect to this line you know; what is the temperature of the inlet and you know; what is the temperature of the heat transfer fluid. So, you fix those things and you fix the reactor temperature corresponding to one of these steady states and we also argued that

when we have these kind of 3 steady states available, when you have 3 steady states available what is happening is that if you are in the top or the bottom these 2 steady states, these are stable steady states because if your moving on this side. So, for example, if you are heating it up, basically your cooling curve which is in black here and which was in blue here is higher than your heating curve.

So, it cools down, comes back, this side also it is the same thing, but if you are looking at this situation, if you heat it up little bit; what will happen is that your heating curve is higher than your cooling curve. So, basically, it will start heating up further until it goes to this particular steady state.

So, when you are operating at these particular line it does not go anywhere else you know it has to be your reaction system has to move somewhere on this particular line itself now we will discuss something more if you look at this particular point here that you see at this particular point the intersection these 2 lines did not cross here they are crossing here, it just touches and goes and here also, although I have not drawn it very clearly, it just touches this line and goes and these point; point number 10.

This is called ignition point why this is ignition point because if you are so basically remember your operating on this line, then you can access this steady state, no problem, it is at this steady state, if you do not disturb its state, it stays there even in the case of an unstable steady state, if you do not disturb the system, it will stay there, but slight disturbance will be need to go to a higher or lower steady state and a reactor that is designed to operate at a particular steady state for a particular conversion if it goes to higher or lower steady state it will not do optimum situation for you. So, you have to be very careful now looking at this particular graph if you look at this particular point what happen if you increase the temperature slightly.

So, if you increase the temperature slightly what happens is that there is no steady state for this system that is remaining nearby which means basically, if you are heating it up slightly, it will spontaneously heat up and it will go all the way to point number 11, this is something that you have to keep in mind so, because you have changed the temperature slightly here. So, if you change the temperature slightly here ultimately it will stay in this line right what are the steady states available in this line the next steady state that is available is here and you know when you have come to this height your heating curve is already higher than your cooling curve.

So, it will now spontaneously heat up until it reaches the steady state because this operating line is defined by this operating line is already defined by your corresponding Tc and T 0. So, if you heat up slightly or if you give slightly more energy it has to go suddenly here now it is not exonerated here, but actually it will be exonerated in real situation in a in a way that I mean these temperature is basically much higher than this particular temperature.

So, which means it will suddenly the reaction mixture will suddenly release lot of heat and the system will go from this point to this point; that means, the reaction temperature will go up suddenly with large heat release this is called then the ignition point the reaction may catch fire also in this particular situation. So, it has to go to a new steady state which will be somewhere here.

So, that is the ignition point for you now if you say for example, if you are considering this particular point here also it just touches this line. So, if it touches this particular line. So, remember, when you are at this point you have heated up slight heating it goes here if you cool down slightly there is no problem because heating curve is higher than the cooling curve. So, then what will happen the system will self correct and then the system will heat up and it comes back to this position, but if you heat up slightly, then there is a problem it has to go all the way to steady state.

So, which means temperature has to increase enormously from this point to this point temperature of the reactor has to increase enormously and; that means, the reaction will release large amount of heat it may ignite it will ignite, but if you are considering this point, for example, if you are at this point. So, this just touches rate line just touches this black line if they are at this point and if you heat up little bit what will happen this black curve is higher than the red curve.

So, basically the cooling rate the heat transfer rate is higher than the heat generation rate. So, it will be cool back spontaneously to this position no problem, but if you cool down little bit, then what will happen if you cool down little bit there is no steady state available close by, it cannot go back here because in order to go back here it has to heat up, but the heat removal line is basically higher than your heat generation line it has to come to another steady state and all the way down along this line there is only one steady state available which is this point.

So, it has to come back to this point; that means the reaction temperature has to decrease from this point to this point. So, large decrease in temperature will occur. So, basically this is called extinction point. So, you will have this kind of you will see this kind of ignition points extinction points it is important to keep in mind which point is ignition point and which point is extinction point you may have real problems.

If you are working near ignition point slightly heating means you may have you may end up in ignition and a accident and a bad situation. So, I hope this has given you a little bit of idea about this kind of you know the multiple steady states and how they basically generate because this is the solution you see one thing when you are having the rate expression here this rate expression is basically small k into a to the; sorry, it has small k into concentration some concentration raised to the power something small k is basically A into e to the power minus E by RT.

So, if you look at this particular term here. So, this term comes in on the left hand side. So, overall the left hand side if the dependence temp on temperature is not linear because the temperature appears in this formed and that will that will explain to you why if your plotting this term as a function of temperature you will have a non-linear graph because this term as a non-linear dependence on temperature because this term this exponential the temperature appears in the exponential term. So, the like this you can generate the graph or these different graphs and you can operate at different multiple steady states I mean you have multiple steady states you can choose the steady states that you like to and it also depends on the consideration that you cannot really choose all the steady states.

So, let me replace this you cannot choose any steady state that you like to because your situation dictates you may not choose the lowest steady state may be conversion is very low now let us elaborate on this little bit further one problem this one is not very good. So, I will just exchange this one problem that I want to discuss here is the is the following.

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So, let us say you are working with a CSTR and with heat exchange; that means, it is an isothermal situation you are working with a reaction A to B; first order reaction liquid state first order reaction the temperature the feed temperature which is T 0 is 20 degree Celsius whatever is the feed we are putting 0 FA 0 T 0 like that and let us say, the reactor temperature is 170 degree Celsius and the temperature of the heat exchange fluid which is Tc is 40 degree Celsius and let us say this reaction is an exothermic reaction.

So, delta H of reaction is minus 30 kilo calorie per mole and the heat capacity of A is equal to the heat capacity of B is 0.15 kilo calorie per mole Kelvin; small k which is the rate constant is equals to 0.8 per hour at 170 degree Celsius because you are doing the reaction 170 degree Celsius; you need this value of k CA 0 that is the concentration reactor feed of A is 3000 moles per metre cube and v 0; small v 0 is the volumetric flow rate in this 0.2 metre cube per hour concentrate on the units you should not make a mistake with the units. Now the question is the first question is; what is the size of the reactor that is required in order to get a ninety percent conversion ok.

So, let us go to the mass balance FA 0 minus FA plus r A V is equals to 0. This is your mass balance all right, what is FA 0? FA 0 is nothing, but CA 0 into volumetric flow in. So, these things are already given just put then 600, it comes out as 600 mole per hour, 600 mole per hour and what is FA; you are talking at 90 percent conversion. So, FA is basically 0.1 into FA 0. So, FA 0 minus 0.1 into FA 0 90 percent

conversion has occurred. So, these 0.1 into FA 0 minus first order rate. So, k into CA into V equals to 0, this V you have to find out now all things are basically given here because the concentration of a concentration of a that was say 3000 if you are looking at the concentration of a that is 3000 that is at the entrance.

So, concentration of a here in the reaction mixture will be point one of CA 0 that is also because ninety percent of conversion has occurred now. So, this will be if you take 1 minus 0.1. So, this will be 0.9 into FA 0; FA 0 is nothing, but 600 moles per hour minus small k. Now small k is 0.8 per hour into CA is 0.1 into CA 0 which is 3000 mole per metre cube into V equals to 0, all right. So, from here what you can find out is the V which is 2.3 metre cube.

Now of course, in doing these you just use the mole balance you did not talk about the energy balance, I mean actually these thing, we have done before also nothing new second question is more interesting; what is the heat transfer coefficient required; what is the heat transfer coefficient small u; remember, small u into A is your heat transfer coefficient needed given that the heat transfer area is 6.13 metre square.

Now something you have to keep in mind heat transfer is very important when you are looking at an exothermic reaction, if you do not take away the heat the reaction may be run away reaction. So, you are trying to take away the heat also it is complicated by the fact that your polymer that is produced many times the polymerisation system that is not conductive.

So, heat cannot be conducted away that easily. So, heat low hotspots can generate and it can create run away reaction. So, it is very important to concentrate on these particular thing efficient heat transfer away with a heat transfer fluid. So, it also depends on the material that you have used to construct the reactor because the heat transfer coefficient is characteristics of that material that multiplied by the area that multiplied by the area of heat transfer that is available with respect to the reactor multiplied by the difference in temperature between the inside of the reactor and the heat transfer fluid.

This is the rate of heat transfer basically, now of course, you want as much area heat transfer area of the reactor as possible and you also want high heat transfer coefficient high heat transfer coefficient depends on the material, but one problem here is that what can happen may be the polymer has been produced and it gets deposited on the surface of the reactor since this is not conductive this can in effect reduced the heat transfer coefficient this is called the reactor fouling; f o u l i n g reactor; fouling, what other thing also you have to consider is that if you have to scale up you have to size up the reactor if the size is becoming bigger and bigger the volume is increasing, but the area or the heat transfer area of the reactor does not increase in the same proportion.

So, when you go to larger and larger sized reactor basically your heat transfer efficiency will decrease. So, when you are engineering this kind of reactors some of these important points you need to keep in mind. So, with respect to that only this problem I hope you might find some importance. So, this is the second part of the problem in order to solve this; this part of the problem, we want to write down the energy balance equation FA 0 into C PA into T minus T 0 equal to delta H reaction FA minus FA 0 plus Q dot. So, if you see the energy balance equation that we had written before.

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So, you see here, this was the energy balance equation for steady state ultimately we came to this situation here, but this was the energy balance equation to start with. So, that is the same thing that I am writing down here. So, FA 0 into C PA minus T 0 equals to this plus the Q dot this part.

So, your FA 0 is already known which is 600 moles per hour C PA is already known heat capacity 0.15 kilo calorie per mole per Kelvin T minus T 0 is already known T is 170

degrees T 0 is 20 delta H reaction is given is the exothermic reaction you put that value FA minus F 0 FA 0 you already know because FA is point one of FA 0 and Q dot Q dot actually.

So, these terms you know, I will not write down these term Q dot basically is your; as you can see this was the Q dot this is the heat transfer coefficient rate of the reactor material into the area of heat transfer into difference in temperature. So, that you write down here uA into Tc minus T all this things are known. In fact, here you have you have to find out these value of u because area of heat transfer also is given and Tc is given what is Tc? Tc is the temperature of the heat transfer fluid this 40 degree Celsius and T is the temperature of the reactor 170 degree Celsius.

So, ultimately from here you can find out the value of u which will be 3.4 kilo calorie per metre square per Kelvin per hour. So, you see this is the heat transfer coefficient per unit area per degree Celsius per unit time. So, if you multiply this by the area, you will get the heat transfer. So, the multiply these by the area; that means, metre square will go and multiply by this temperature difference, then the Kelvin will go. So, ultimately, it will be the heat transfer; total heat transfer that will be your kilo calorie per hour, right that will be kilo calorie per hour.

So, this is how we solve I mean for the first part you just let them mole balance for the second part you needed the energy balance and this is the energy balance equation that you are going to use and basically it is this particular expression, all right. So, now, what we are going to do is the following before I finish off the discussion on the reactors I will be a doing a couple of more problems and that is the end of our discussion on the on the reactors.

So, I mean just to give you more idea about the steady state situation because steady states situation how to talk about this multiple steady states this thing we have not discussed with a problem.

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So, I thought that we might discuss that as per as this is concerned. So, let us define the problem let us say we are working with a CSTR and we have a reaction which is A plus B which goes to C. Now for this particular system, certain things are given to you and what are those things heat capacity of a is hundred 80 joules per Kelvin per mole heat capacity of B is 80 joules per Kelvin per mole the temperature at the inlet T 0 is 290 Kelvin and the volumetric flow in is eight metre cube per hour and flow rate in of each component flow rate in I mean the inlet flow rate for each component is 100 moles per hour and the rate of the reaction is basically first order in A and 0 th order in B just to simplify the matter, all right.

The reaction is exothermic with the heat of reaction minus 60,000 joules per mole the heat transfer coefficient times the heat transfer area is 1 into 10 to the power four joules per hour per Kelvin what else is remaining the temperature of the coolant fluid is 310 Kelvin. So, we are defining the problem. Now you have not yet started solving because we do not know what to solve have not yet told you what we want to solve and the rate constant this is very important you need to know this as a function of temperature 10 to the power 10 into e to the power minus 80,000 divided by RT per hour.

So, all these things are given along with that also the volume of the reactor is given you are doing the reaction in CSTR which has a volume of twenty metre cube. Now I hope

the definition of the problem is complete, all right. So, what we want to know is that for this particular system.

So, you are doing the reaction a plus b equals to c this is the rate law and this is the rate constant how it varies with temperature and these are the different heat capacity values that you have and these are the respective temperatures of the heat transfer fluid and the inlet temperature and the volumetric flow rate and the molar flow rate in this molar flow in all are given and this is the delta H that is the enthalpy change for the reaction is also given heat transfer area into heat transfer coefficient is also given CSTR volume is given.

So, the question is; what are the steady state operating conditions under this situation what are the steady state operating conditions. So, what you do you write down your expression of the steady state here. So, 0; so, there is no heat accumulation is equals to minus FA 0. So, you see here FA 0 into C PA into T minus T 0, but here this instant of C PA you have to add this C PA plus C PB because A and B both are there.

So, it will be FA 0 minus FA 0 C PA plus FB 0 C PB into T minus T 0 plus delta H of reaction into r A into V plus uA into Tc minus T its a second thing. So, you just take this term on this side and Q dot is basically Q dot is basically this thing and this side is 0. Now you know the value of FA 0 is the same as value of FB 0 which is 100 moles per hour and this C PA. So, this FA 0 comes out and C PA plus C PB is basically C PA is hundred 80 C PB is 80 and then you divide all through FA 0 by then what you will get you will get 0 equals to minus.

So, this C PA plus C PB is 250 into T minus T 0. T 0 is 290; 290 plus delta H of reaction is minus 60,000. So, there is minus 60,000. Now r A V divided by FA 0 is nothing, but minus x that is the minus of conversion, we have already talked about that because conversion is FA 0 minus FA by FA 0 then r A V is FA 0 minus FA minus of that. So, is the term here, now plus uA into Tc minus T divided by FA 0. So, what is the term uA divided by FA 0 you know all these things your uA is 10 thousand 10 thousand divided by FA 0 is your hundred the units if you consider you have to consider the units also.

So, ultimately what you will get here is this will be hundred joules per mole Kelvin hundred joules per mole Kelvin uA by FA 0. So, that uA by FA 0 will be here. So, that will be hundred into Tc temperature of the fluid or heat transfer fluid that will be 300 temperature of the heat transfer fluid is, sorry, it is not 300 it is 310; 310 minus T.

So, from here what you will get. So, from the energy balance we have done the energy balance here. So, what you will get is this term x equal to minus 1.725 plus 0.00583 t. So, what you got is basically your conversion as a function of temperature it is a straight line from this linear equation you will get this particular curve this is also true because you are taking away the energy from the system.

So, when you are taking away the energy from the system you have this coolant liquid information here uA, this information here. So, it is this height that am going to talk about it is this height you can plot this height as a function of temperature and you can get this kind of linear plot or you could plot x as a function of temperature and you can get a linear plot about this side that I was telling that I will tell after because that is also very important this kind of curved line you can get when x is a function of T in a non-linear fashion right in that expression of x you can get e to the power minus e by RT and that is why that nonlinearity is coming when you are coming from the right hand side you do not see that non-linearity you understand the point here.

So, you take this energy balance equation and you get ultimately this expression of x and if you plot this as a function of T it is a linear plot it is a linear plot. So, you are going to get these kind of plot now if you do a mass balance remember in this on the left side, I got confused about if you look at the left side this x basically you can replace by your expression of rate because that is expression is coming from the mass balance there that nonlinearity is coming that minus e by RT and there you are getting this kind of curve. So, for energy balance although this is your steady state equation if you are going to plot conversion as a function of T just do the energy balance and you will get x as a function of T in a linear fashion and. Secondly, now you do the mass balance.

If you are going to do the mass balance here what you will get 0 equals to FA 0 minus FA plus r A V, right. So, 0 equals to FA 0 minus FA is volumetric flow volumetric flow into concentration of a volumetric flow out it will be equal to the volumetric flow in steady state situation now r A is basically k into CA ka into CA or k into CA whatever way you want to show it into V from here you get an expression of CA which is FA 0 divided by V plus kV. Now FA is V into CA and you know the expression of CA is already here. So, if you put that expression of CA and take the V down you will get FA 0 divided by one plus small k into capital V by small v. Now this capital V by small v is your tau which is your residence time. So, 1 plus k tau.

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So, now if we use this expression in the expression of x it is FA 0 minus FA divided by FA 0 and you put this value of FA here ultimately what you will get is k tau divided by one plus k tau this is what I was talking about this k tau. So, when you are applying the mass balance equation that mass balance equation you could apply to this particular side this x you could get the expression of x from here and you can replace that expression of x here and then you are getting a non-linear curve non-linear curve because in the expression of x there is this small k and this small k varies with temperature that exponential term is there where it is like this.

So, you have this term. So, from here how do you know all the values you know the value of k small k which is this term this expression this expression and you also know value of tau what is the value of tau capital V by small v. So, value of tau is capital V by small v which is 20 divided by 8 which is 2.5 hour. So, what you do you put 2.5 here and small k is there with respect to t.

So, you can plot these x as a function of T and this will give you the non-linear curve or an equivalent of the GT verses T curve and this will give you the linear curve and equivalent of RT verses T curve. So, you can plot this thing in excel by changing the temperature very easily. So, if you plot this expression and this expression you get a linear curve and you get a GT curve. So, this is something that I have done for you I have plotted in excel. (Refer Slide Time: 34:56)



So, if you go the power point slide. So, you will see this black curve which is the linear dependence of conversion on reactor temperature that appears from the energy balance equation do not go by the general energy balance equation that I had shown before because the general energy balance equation at one side minus delta H reaction into x and on another side you have pa into one plus tau kappa into minus T prime.

So, general energy balance equation that shows you the balance one side is GT one side is RT that is all now you can take the RT and plot against the you get a linear curve or a you can take the GT against T, you get a linear curve that is all, but what we are doing here is that we just take the energy balance equation and from there we get the expression of the conversion as a function of T that will be a linear term that will be a straight line and when we get the conversion as a function of T that is temperature by applying mole balance you will get a non-linear dependence because there the small k will come.

So, mole balance and energy balance are different that way. So, if you now come back to the power point slide. So, this black curve has been generated by getting the value of x as a function of temperature this is reactor temperature in Kelvin and this is conversion x as a function of temperature. So, this is a linear curve and this rate curve is basically your x equals to k tau by 1 plus k tau that we have got and tau value we know this is this tau value is how much 2.5 hours and small k actually has a temperature term.

So, you can very easily plot that in excel and you will get a rate curve like this; this is from the mole balance and this black curve is from the energy balance. So, this is straight line and this is curved line this is a very similar situation to if you just plotted the GT the rate of heat generation as a function of T then also you will get the same curve if you just plotted the RT the rate of heat removal as a function of T then you will get a black curve. So, for the problem I have discussed if you just go to the previous energy balance equation where GT equals RT you have derived if you if you take that expression of GT and if you plot against you will get these curve.

So, you can work it out by yourself. So, the point is here you have 3 intersection this is one point of intersection this is one point of intersection and this is another point of intersection 3 points of intersection and we have I have worked this out if you if you come back to the script here I have worked this out those 3 points of intersection are at 3 different temperatures of the reactors and the corresponding conversions also have worked out.

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So, 296, 0.00019, 417.3, 0.71 and 459.2; 0.95; so, basically you have 3 steady state situations, either you can operate at this temperature when you will get this conversion this temperature or this conversion or this temperature, this conversion, you see at what temperature, you do not want to operate very low conversion may be you can operate at the middle temperature point seven one technologically important polymers you can get

or at a higher temperature. So, this is how you can solve this kind of problems and you can get the multiple steady state situations depending on the parameters that we have got.

So, what we will do in the next class is very briefly, we will talk about a situation where we are going to work with polymers for the same problem and we are going to have a some simplifying assumptions and this kind of steady states situations we can all we can derive by following the same kind of logic and approach and then we will start talking about the synthesis of the different industrial polymers. So, till then.

Thank you and good bye.