Principles of Polymer Synthesis
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Lecture - 31
Design of Chemical Reactors (Contd.)

Welcome back for the 7th week of this lecture series on my NPTEL course on principles of polymer synthesis. Over the last week or so we have been talking about principles of chemical reactor design. And if you remember towards the end of the last week, we discussed about the CSTR steady state multiplicity, and we also try to solve some problems.

So, today is the last class as far as the chemical reactor concept is concerned, after that we will go into the synthesis of commercially important step growth polymers. So, let us do maybe a couple of more problems before we finish this topic on the design of chemical reactors.

So, if you remember, last week we finished with this particular problem here.

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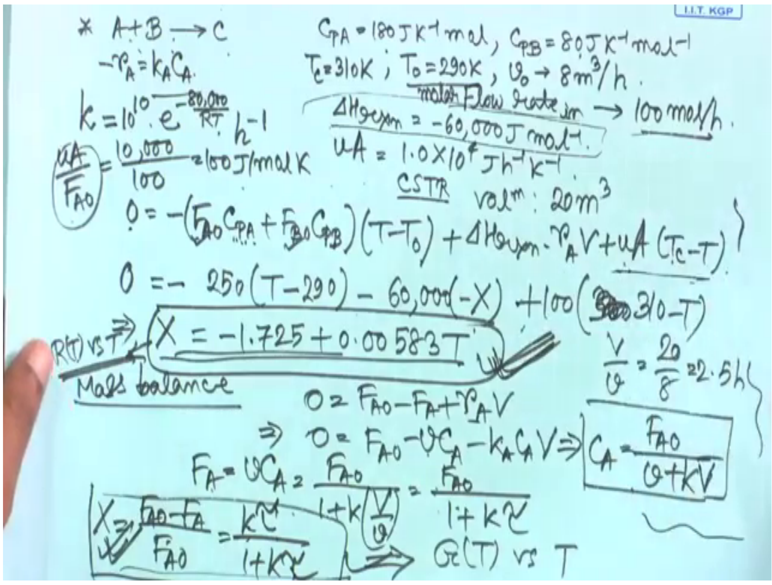

* $A + B \rightarrow C$

$-r_A = k_A C_A$

$k = 10^{10} \cdot e^{-\frac{80,000}{RT}}\ h^{-1}$

$\frac{uA}{F_{A0}} = \frac{10,000}{100} = 100\ J/mol\ K$

$C_{PA} = 180\ J K^{-1} mol$, $C_{PB} = 80\ J K^{-1} mol^{-1}$

$T_c = 310 K$; $T_0 = 290 K$, $\upsilon_0 \rightarrow 8 m^3/h$.

molar flow rate in $\rightarrow$ 100 mol/h .

$\Delta H_{rxn} = -60,000\ J\ mol^{-1}$.

$uA = 1.0 \times 10^4\ J h^{-1} K^{-1}$

CSTR vol^m : $20 m^3$

$$0 = -(F_{A0}C_{PA} + F_{B0}C_{PB})(T - T_0) + \Delta H_{rxn} \cdot r_A V + uA(T_c - T)$$

$$0 = -250(T - 290) - 60,000(-X) + 100(310 - T)$$

R(T) vs T $\Rightarrow$ $\boxed{X = -1.725 + 0.00583T}$

$\frac{V}{\upsilon} = \frac{20}{8} = 2.5 h$

Mass balance

$$0 = F_{A0} - F_A + r_A V$$

$$\Rightarrow 0 = F_{A0} - \upsilon C_A - k_A C_A V \Rightarrow \boxed{C_A = \frac{F_{A0}}{\upsilon + kV}}$$

$$F_A = \upsilon C_A = \frac{F_{A0}}{1 + k\left(\frac{V}{\upsilon}\right)} = \frac{F_{A0}}{1 + k\tau}$$

$$\boxed{X = \frac{F_{A0} - F_A}{F_{A0}} = \frac{k\tau}{1 + k\tau}} \Rightarrow G(T) \text{ vs } T$$

So, we took some reaction say A plus B goes to C, and the rate equation is also given for simplicity, it is first order in A and 0th order in B. And the rate constant was given as a function of temperature. And also, some other information were given like the heat capacity of the respective reacting species, it was also assumed that the heat capacity is constant which temperature does not change.

The temperature of the heat transfer fluid temperature of the inlet volumetric flow rate in and molar flow rate in all these things were given and delta H of reaction that is the enthalpy of reaction was given minus. So, it is exothermic reaction also the heat transfer characteristics were given.

If you remember u is basically the heat transfer coefficient of the material of construction of the reactor. And A is basically the area over which the heat transfer occurs. CSTR volume was also given. So, the question was find the steady state operating conditions. And we used this energy balance equation in the steady state for CSTR to find out, X that is the conversion as a function of temperature directly.

So, this was linear, and then what we also do is separately we apply mole balance to the expression of conversion, and what we find is the variation of X as a function of temperature. And there it is not linear because the small k the rate constant contains the temperature in the exponential form. E to the power minus activation energy divided by r into T and then the intersection of these 2 graphs will give you the solutions in this case there are 3 intersections. So, there are basically 3 solutions.

So, what I will do today is to do the same problem again, but for a polymerization reaction an exothermic polymerization reaction specifically, the polymerization of styrene. And we are going to have some assumptions that are going to simplify our problem. You have to remember that in reality the problem will be a little bit more complex, but just to give you a correlation with the concepts that we have shown here. I would like to solve that problem with those nevertheless with those simplified assumptions put in place.

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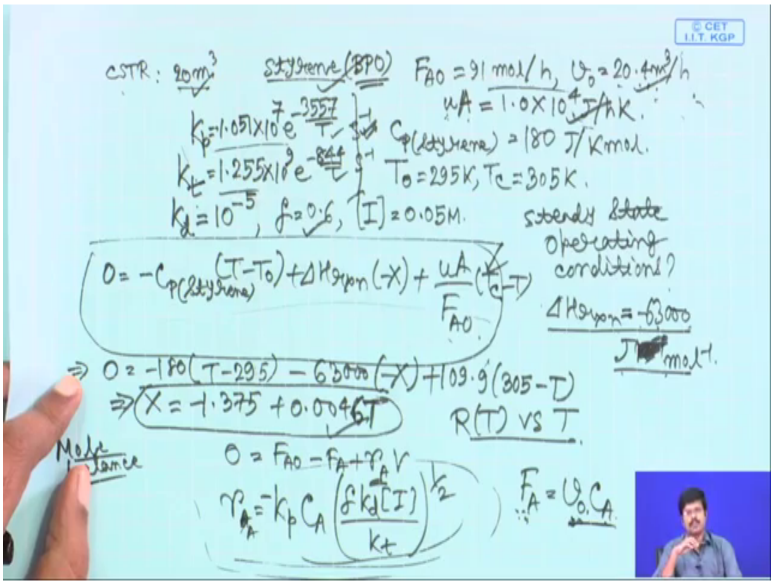

CSTR : $20 m^3$ styrene (BPO) $F_{A0} = 91$ mol/h, $\upsilon_0 = 20.4 m^3/h$

$uA = 1.0 \times 10^4$ J/hK.

$k_p = 1.051 \times 10^7 e^{-\frac{3557}{T}}$ s^{-1}

$C_{p(styrene)} = 180$ J/K mol.

$k_t = 1.255 \times 10^9 e^{-\frac{844}{T}}$ s^{-1}

$T_0 = 295 K, T_c = 305 K.$

$k_d = 10^{-5}$, $f = 0.6$, $[I] = 0.05 M$.

steady state operating conditions?

$$0 = -C_{p(styrene)}(T - T_0) + \Delta H_{rxn}(-X) + \frac{uA}{F_{A0}}(T_c - T)$$

$\Delta H_{rxn} = -63000$ J [illegible] mol^{-1}.

$$\Rightarrow 0 = -180(T - 295) - 63000(-X) + 109.9(305 - T)$$

$$\Rightarrow X = -1.375 + 0.0046T$$

R(T) vs T

Mole balance

$$0 = F_{A0} - F_A + r_A V$$

$$r_A = -k_p C_A \left(\frac{f k_d [I]}{k_t}\right)^{1/2}$$

$F_A = \upsilon_0 C_A$

So, let us have the definition of the problem then. So, the problem is something like this. Let us say we have a CSTR, continuous start tank reactor which has a volume of 20-meter cube. And you are polymerizing styrene in this reactor. And what is given is the following the molar flow rate in is given is that is 91 moles per hour. And also, the volumetric flow rate is given, which is 24.4-meter cube per hour.

Now, these things have optimized for to demonstrate the concept that I have already shown in the previous problem. Now these things of course, you can also control this is user controlled. And the heat transfer characteristics is like this uA u into A u is the heat transfer coefficient a is the area over which the heat transfer occurs. That is equal to 1 into 10 to the power 4 joules per hour Kelvin.

Now, some of the data I have taken from literature like the heat capacity of styrene. Heat capacity of styrene is equal to 180 joules per Kelvin per mole. T 0 this again I am defining say T 0 is the inlet temperature; let us say that is 295 Kelvin. And Tc is the temperature of the heat transfer fluid which is 305 Kelvin. And again, from the literature for the styrene polymerization the kp is something like, this is the rate constant for propagation this kp the value is 1.051 into 10 to the power 7 e to the power minus 3 5 5 7 divided by T ok. And kt which is the termination rate constant which will be orders of magnitude higher than the propagation rate constant.

If you remember, our discussion on the principle of radical polymerization we had mentioned that, and indeed this is so 1.255 in this case, it is 2 orders of magnitude higher

10 to the power 9 e to the power minus 8; 44 divided by T. And kd that is the dissociation constant for the initiator we are assuming that in this case, we are using benzoyl peroxide as initiator.

Now, kd is very small. It also has a dependence on temperature, but for simplicity again I am just assuming it is constant at 10 to the power minus 5; now small f which is the initiator efficiency. Let us assume it is 0.6. And let us say the initiator concentration is 0.5 molar.

Now, remember, in actuality the situation will be the situation will be little bit more complex because, your efficiency of the initiator also can change with the progressive polymerization. Not only that the initiative concentration can also drop with the progress of polymerization. And this kp and kt, if you remember, the concept of auto acceleration, what can happen is that with the progress of polymerization your kp will decrease your kt will decrease, but kt will decrease much more so that the rate of polymerization may increase significantly. Those things we are not taking into account we could things will become more complicated. It has to be the situation has to be approached differently. Those things we would not discuss just to have a parallel connection with the previous problem, I brought in this polymerization situation into the scheme of things. And assuming some of these simplified things, and this kp and k T these are literature values the initial stages of conversion, they will be having this kind of dependence ok.

So, with these simplified assumptions we will progress. So, the question then is find the steady state operating conditions. So, what are the steady state operating conditions? So, this is the question. So, we will do the same that we had done for the previous example. So, you will go to the energy balance, and from the energy balance we will get the conversion as a function of temperature the linear function. And then what we will do separately we will apply a mole balance to the conversion. And we will get the dependence on temperature which will be non-linear, and then the intersection of these 2 graphs will give you the solution if it is one intersection then there is only one steady state available under this situation, if there are 2 then there are 2 steady states available. And typically, you would not get more than 3 intersections. So, the maximum number of solutions that you can get are 3.

So, steady state operating conditions and if you remember in the previous example, we had 3 steady state operating conditions. We obtained 3 steady state operating conditions as the solution of the problem. And if you remember, we had shown if you look at the graph in the slide in the PowerPoint slide, we had shown this thing in the graph that energy balance and mole balance equation.

So, the energy balance and the mole balance. So, these 2-energy balance is basically the conversion as a function of temperature that we obtained from the from the energy balance equation.

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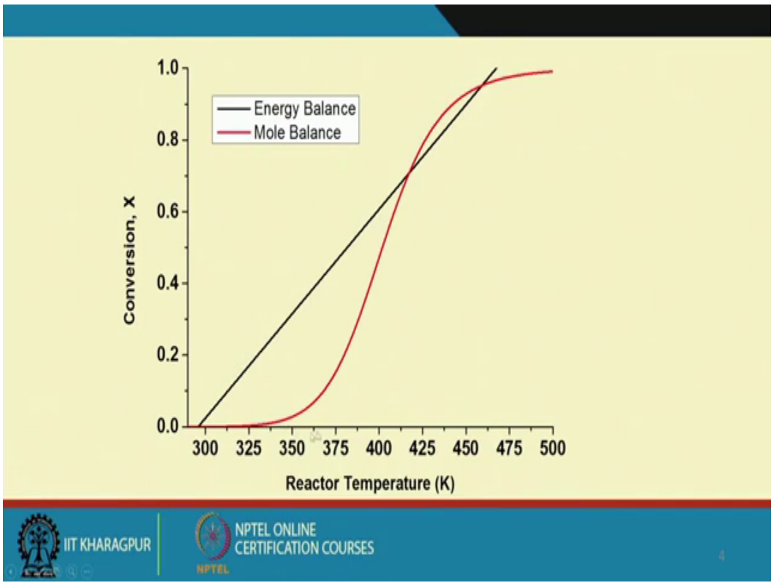

So, that is what we are plotting against the reactor temperature and the rate curve is basically again conversion as a function of temperature, but we are using the mole balance equation that is why it is non-linear. The exponential term is there and basically you have 3 intersections they are; so, which gave you 3 solutions. So, each intersection corresponds to a particular reactor temperature and a particular conversion.

So, if you are working at that particular point, the steady state you are fixing the reactor temperature and you are getting a specific conversion, and as you know under the working conditions in steady state the conversion of the of the CSTR, it does not change it remains same. So, this is what we had solved before. So now, this is the problem that we are going to solve.

So, again for the energy balance, this is steady state energy balance. So, 0 equals to minus CP of styrene into T minus T 0 plus delta H reaction into minus X plus uA divided by FA 0. This is the equation if you remember, if you do not you can just go back and recapitulate this is the original equation. So, whatever number of reactants are there you just add the heat capacities, and we are assuming that the molar flow rate is the same for all the reactants, in this case we have only one reactant though.

So, you put all these values there and then you divide by your molar flow rate. And so, that will be coming here. So, it will be u a Tc minus T divided by FA 0 exactly; that is, what we are putting here. So, this is basically Tc minus T ok. So, if you put the values in there. So, it will be 0 equals to minus 180 into T minus T 0 is 295 minus ok. One more value has to be given for u which is delta H reaction. It is exothermic reactions styrene polymerization vinyl monomers from the polymerize, they will typically polymerize exothermically a lot of heat will be generated. So, delta H reaction here this is again from the literature, that I had obtained is, minus 63,000, minus 63,000 joule per Kelvin, joule per Kelvin per mole. In fact, it is not joule per Kelvin, it is joule per mole excuse me.

So, this is delta H reaction minus 63,000 joules per mole. And the value of uA is also given. So, we can proceed. So, this is 63,000 into minus X plus you just put the values of uA and FA is 0 and mind the units, the Tc is also known. So, if you put all these things, then you will get something like this 109.9 into 305 minus T. So, from here I mean according to what I have calculated, I have already worked out the problem. I do not want to (Refer Time: 12:31) and calculate here.

So, it is minus 1.375. Of course, you can figure it out yourself how the calculations are proceeding after when you look at it with some time in hand. So, this is; so, as a function of temperature, then you have the energy balance equation. So, this will give you a linear plot which is basically equivalent to your RT versus d plot.

So, this you can plot, now the second thing is little bit more involved if you are going for the mole balance equation. Remember, that accumulation is equals to molar flow rate in, minus molar flow rate out plus r A into v. Now from this equation if you remember, what we had taught before the rate of polymerization is basically equals to, I mean, in this case I am putting r A or r.

Let us say A is the styrene whatever. So, rate of polymerization is your rate constant. Basically, it will be negative because this is rate of disappearance of the monomer, into the monomer concentration into small f into kd into I divided by k T to the power half. This is something that we had derived before just right at the start of the discussion of the radical polymerizations. And so, this is the expression that you can use then in this equation.

So, if you use this expression, then what do we get? So, just replace the r here with this expression. And then, also remember that your FA is basically v 0 into concentration of A. So, molar flow rate out, in this case this is molar flow rate out is equals to volumetric flow rate into concentration of A; which is the this is concentration of A, or the concentration of styrene in the reaction mixture, which is constant because it is operating in steady state.

Now, v 0 v 0 is basically the molar flow rate is the volumetric flow rate in that is why the 0 is there. So, inlet volumetric flow rate now this is also equal to the outlet volumetric flow rate, because both are equal in the case of liquid state reactions under steady state conditions. That is why I am putting v 0 here, even though this is the molar flow rate out. So, just put those values in here. So, if you put that value here, and all right. Let me not skip the step, let us go back to this.

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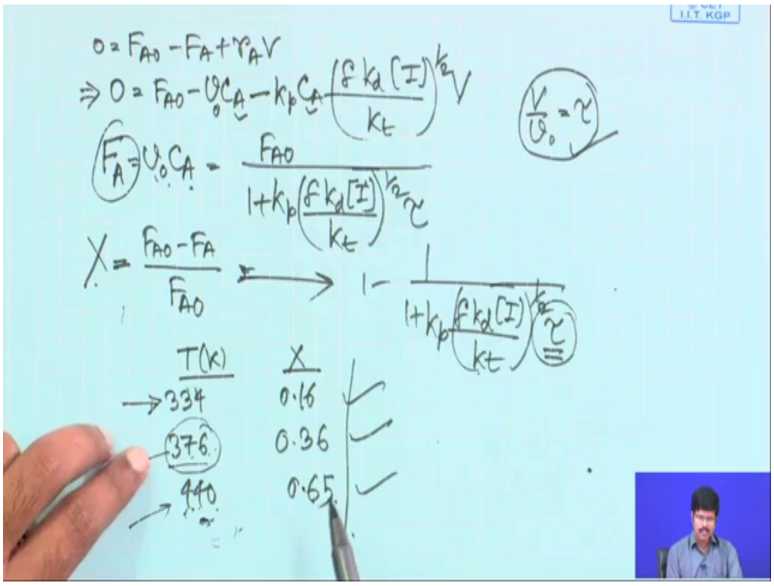

$$0 = F_{A0} - F_A + r_A V$$

$$\Rightarrow 0 = F_{A0} - v_0 C_A - k_p C_A \left(\frac{f k_d [I]}{k_t}\right)^{1/2} V$$

$$\frac{V}{v_0} = \tau$$

$$F_A = v_0 C_A = \frac{F_{A0}}{1 + k_p \left(\frac{f k_d [I]}{k_t}\right)^{1/2} \tau}$$

$$X = \frac{F_{A0} - F_A}{F_{A0}} \longrightarrow 1 - \frac{1}{1 + k_p \left(\frac{f k_d [I]}{k_t}\right)^{1/2} \tau}$$

T(K)	X
334	0.16
376	0.36
440	0.65

If you skip steps, you may commit always mistakes. It is possible not always possible to find a mistake at the moment about doing the math.

So, FA 0 minus v into C A so that is minus v into CA or v 0 into CA minus kp into CA into f kt I divided by k T to the power half into v. And also remember that v by v 0 is basically your residence time. So, if you take that into account and then you can get an expression of CA from here and if you remember again that FA is basically v 0 into CA. Then you can replace the expression of CA from here, and the final expression that you will get is something like this FA 0 divided by 1 plus k p into f kt I divided by k T to the power half into tau.

I mean I just summarized this for you can figure it out yourself. So, this is tau because v 0 into C A. So, basically CA is FA 0 divided by this, v 0 plus this into capital v. Now when you are multiplying by v 0, your v 0 is coming here that v 0 if you take down. So, v 0 v 0 it becomes 1 and this capital V by small v 0 which becomes tau. So, this is your expression.

Now, if you remember, that your conversion in terms of the molar flow rate in and molar flow rate out is basically equal to FA 0 minus FA divided by FA 0. And then if you replace the expression of FA from here, then finally, finally, what you will get is X equals to 1 minus 1 divided by 1 plus k p into f kt I divided by k T to the power half into tau.

So, this gives you the dependence of X on temperature from your mole balance equation. And remember here that this tau is basically known for you, because you already know the volumetric flow rate in. And you already know the volume of the CSTR. So, this divided by this is your tau. And let us see. So, if you look at the expression here, also look at the units it is a power ah. So, basically this is, if you remember correctly this is per second. So, if you have the unit here, per second when you are bringing those expressions here ultimately there will be a per second term remaining.

So, basically have to multiply by 3,600 because you have to go to per hour and that is also because a tau is in terms of hour, because this is 20-meter cube divided by 24.4-meter cube per hour. So, those things you have to keep in mind. Otherwise, you will not get a correct result. And you know the value of ikd etcetera all these things you know.

So, you basically can have an expression of X in terms of T, and although I will not show you the graph that I have plotted unlike the previous problem; where I had shown in the graph, but I will just write down the result for you. So, this is the result basically it has 3 solutions. So, you have 3 steady state, conditions operating conditions that you can choose from. So, 334 370 and 4 for 4 40 Kelvin; these are the 3 temperatures and at these 3 temperatures if you are operating the corresponding conversions 0.16, 16 percent, 0.36, 36 percent 0.65, 65 percent.

So, you have these 3-steady state operating conditions that you can choose from at that particular inlet temperature at all those fixed temperatures that we have. So, inlet temperature is fixed. Your heat transfer fluid temperature is fixed your uA which is your heat transfer coefficient multiplied by the area of heat transfer those things are fixed. And then you can have this solution and. Something you have to remember of course, this is a simplified thing because you know, we didn't did not take into account auto acceleration, and what not, but something you need to keep in mind that oftentimes your the lowest temperature that you can operate in the conversion may be very, very small. So, small that your the molecular weight that you are going to get at the end is not industrially very important. So, you may need to operate in the middle steady state or the higher steady state.

Now, remember that this is the unstable steady state in these kind of situations. These 2 are stable steady states. Now typically in this middle steady static you are operating you will get say 25 percent to 30 percent of the yield per reaction pass. So, if you are looking at that that will be good enough as far as the industrial grade polymer is concerned for this kind of situations say radical polymerization if you are doing say styrene polymerization if you are doing. So, you could also tell that I would go to very high temperature, and then I can get very high conversion. So, one problem there is that oftentimes, this temperature that you have may be quite close to your ceiling temperature. So, that is a problem to do the reaction in, and also you are doing the reaction at a high temperature and remember that it is an exothermic reaction.

So, the safety is also an issue. So, these things you need to keep in mind. And also, something that I showed before, if you if you increase the temperature of your reaction, what can happen is that your degree of polymerization, and hence the molecular weight of the polymer might decrease, I mean I am talking about thermally initiated radical polymerization.

So, those are the things that you need to consider when you are thinking about which steady state to use. Now something else that I wanted to also mentioned here is that, you have; so, this is the problem that I have already solved. So, that is the end of it. So, let us go back and discuss something here as far as the energy balance equation is concerned under steady state, something that you need to keep in mind.

Now, your CSTR may be operated in isothermal condition, or it could be operated in an adiabatic condition, or it could be operated in a non-isothermal condition. You need to be able to differentiate between the 3. So, if you go back to the equations in the script. It is easier to understand why. So, you have this expression here. Now in the in the simplest of terms let me see if I can locate in the previous week, what I had derived for you. So, as far as the energy balance expression was concerned. So, so this is here is one expression that I have got for you say for example, you have this expression, I mean this Q dot is basically this.

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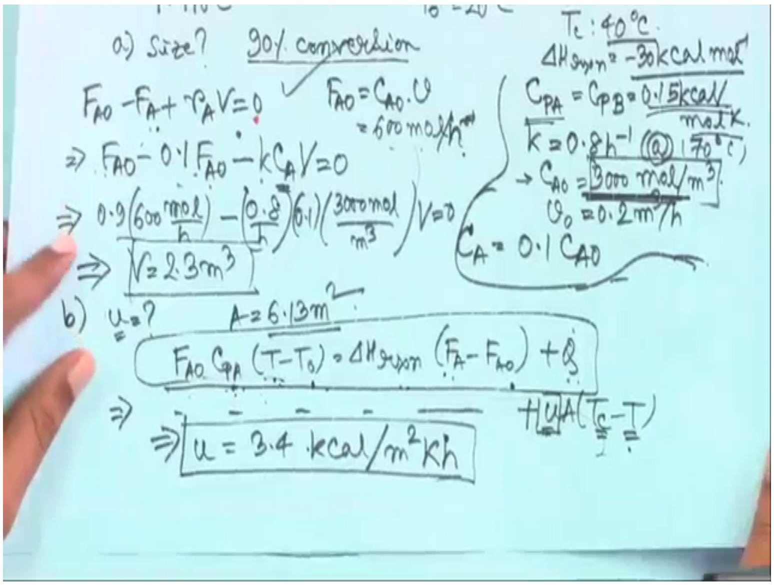

a) Size? 90% conversion

$F_{A0} - F_A + r_A V = 0$ ✓ $F_{A0} = C_{A0} \cdot \upsilon = 600\ mol/h$

$\Rightarrow F_{A0} - 0.1 F_{A0} - k C_A V = 0$

$\Rightarrow 0.9 \left(600 \frac{mol}{h}\right) - \left(\frac{0.8}{h}\right)(0.1)\left(\frac{3000\ mol}{m^3}\right) V = 0$

$\Rightarrow \boxed{V = 2.3\ m^3}$

$T_c : 40^\circ C$

$\Delta H_{rxn} = -30\ kcal\ mol^{-1}$

$C_{PA} = C_{PB} = 0.15\ kcal/mol\,K$

$k = 0.8\ h^{-1}$ @ $(70^\circ C)$

$\rightarrow C_{A0} = \boxed{3000\ mol/m^3}$

$\upsilon_0 = 0.2\ m^3/h$

$C_A = 0.1\ C_{A0}$

b) $U = ?$ $A = 6.13\ m^2$

$$\boxed{F_{A0} C_{PA} (T - T_0) = \Delta H_{rxn} (F_A - F_{A0}) + \dot{Q}}$$

$+ UA(T_c - T)$

$\Rightarrow \boxed{U = 3.4\ kcal/m^2 K h}$

So, Q dot is basically this term. Now I mean if you have to directly plot say RT versus T. Remember that you when you are plotting your X versus T that you have got from the energy balance equation that gives you an equivalent of RT versus T, but if you are asked to plot the rate of heat taken away as a function of reactor temperature. That is the RT versus T, or you are asked to plot g T versus T that is the rate of heat generated as a function of temperature. You can you can directly go to this particular equation the steady state.

So, if you look at this particular equation. So, this part so, this part basically will give you the; you know the rate of heat generated. So, if you look at this particular term, it is basically the same as this particular expression, in different forms they are. So, if you look at this particular expression here. So, this part, will you that the rate of heat generated as a function of temperature because the temperature term will come here. Because you know this is this you can express in terms of X if you remember. So, that will be minus of X when you divide by FA 0 ok So that that is the term then you can directly take, because that will give you the gt as a function of T and then you can plot against T.

Now, if you take this term on this side, then collectively this term minus Q dot that term will give you the RT versus T plot. Now of course, you divide by FA 0 that side also. So, it will be cpa into T minus T 0 minus Q dot divided by FA 0, you take this term on this side, and you divide whole through by FA 0. So, that term. So, this minus this will then give you the RT versus T curve.

Now, if you are if you are looking at your expression, then I mean it is this expression is basically the same as this expression. So, if you are working under isothermal condition, something that you need to keep in mind if you are working under isothermal condition, then what will happen is that your inlet temperature will be equal to the temperature in the reaction mixture. So, basically then this term will go. So, you are only left with these 2 terms in this case.

So, if you are working in isothermal steady state situation then this term will go T equals to T 0. And if you are working in adiabatic situation adiabatic situation is a situation where there is no heat exchange with the surroundings. So, then this heat transfer term will go. So, those things you need to keep in mind. So, the situation that we are working in although you are keeping the temperature of the reaction mixture constant. Strictly speaking it is something different from your typical isothermal situation that we talked about because it is T is not equals to T 0.

So, basically you are operating in a non-isothermal condition. Because remember, that if it were isothermal situation, your temperature of the reaction mixture will not rise in the first place. As far as it is it is value with respect to the inlet temperature is concerned. So, you have allowed the temperature rise to a certain extent the difference being T minus T 0 T being the reactor temperature and T 0 being a temperature at the inlet.

Now, and then you are maintaining this difference in temperature by taking away the heat from the reaction mixture by using a heat transfer fluid, that is the idea. So, you are operating in a situation, whether your temperature of the reaction mixture is higher than the temperature of the inlet. Or so, this particular situation is not your adiabatic situation, because you are taking away heat. So, when you are operating in an adiabatic condition in a steady state condition basically you are not having any heat exchange. So, the heat transfer term will become 0. So, if you asked a problem where you are told that the CSTR is operating in isothermal condition, then that particular term where T minus T 0 is there that term goes to 0 because T equals T 0.

If you are asked about the problem to find about steadies there about information on the steady states adiabatic situation the heat transfer away the term uA into this T minus Tc minus T that term becomes 0. So, those things you need to you need to keep in mind. So, so, that is it overall that is what I wanted to discuss as far as this particular thing regarding the reactors are concerned.

Now, in a nutshell, let us try to summarize certain things. So, if you remember from the start what we had done is basically the same. So, we are now trying to summarize what we have learnt about the chemical reactors. So, basically, we talked about flow reactors we talked about batch reactor. So, the among the flow reactors we talked about different kinds of flow reactors like plug flow reactor like CSTR which is continuously stirred tank reactor. And also, we talked about batch reactor which is different which is not a flow reactor.

And remember, that other than plug flow reactor we also talked about packed bed reactor which is also a kind of flow reactor. And they have different design equations, and these things we discussed, and the design equations initially we derived from simple consideration of mole balance in steady state condition. And afterwards what we also argued is that we need to express these design equations in terms of the actual conversions that you are targeting for a particular chemical reaction to be conducted in that reactor.

So, that ultimately the design equation will contain the expression in this expression the conversion. And then for a targeted conversion in the particular steady state you can know for example, how long you have to keep it in a batch reactor because you are not taking out anything as long as the reaction is going on. We have done this kind of problem also during the progress of this course. And if you are in a flow reactor for example, in a CSTR then you have to know the volume, because the volume controls the conversion and not the time. Because the time is fixed that way. And it is a steady state situation. And of course, there is a term which is the residence time, if you can increase the residence time. If you increase the residence time which means your reactants are there for more time in the in the CSTR; that means, there is more conversion correspondingly so on and so forth.

So, those things you need to keep in mind. These are intricate some of the intricate details, but things are simple in general. So, we also told that when you are expressing the design equation in terms of conversion, what we need to know is the rate law in terms of conversion. Because otherwise we cannot correlate the things. So, what we did also then we went back and we did some simple what may look like simple physical chemistry classes, we derived the rate law we we did if I remember correctly one one simple problem regarding the derivation of rate laws.

So, the rate law will give you the rate as a function of the concentration of different species that are present. And then what you have to do those concentrations. So, different species you have to express in terms of conversion, and that is your stochiometric symmetric table. And by combining your rate law with a stochiometric table, you can get ultimately the expression of rate as a function of conversion.

So, then this expression of rate is there in your design equation. So, you replace that expression with the function with the conversion and then you have your final design equation. So, those things we discussed. And afterwards we also discussed some details regarding CSTR and PFR in terms of if you are aiming for a particular conversion whether you are going to use more than one CSTR, or if you can use only one CSTR we argued, that if you split up say you are going for 80 percent conversion if you use 2

CSTRs maybe in the first CSTR you get 40 percent, and then that you take in the inlet of the second CSTR. And you go for 80 percent finally, then a total volume necessary will be lower.

We also discussed this graphically we also showed this mathematic mathematically. And then also we talked about PFR plug flow reactor. And we did the same problem, and we told it is the area under the levenspiel plot that gives you the total volume necessary for the PFA PFR to get a specific conversion. And then you have to solve an integral, and in order to solve that integral you may need to have numerical approach. So, we also discuss things like trapezoidal rule simpsons one third rule simpsons 3 8h rule, and did some simple problems related to that in actuality. If I am asking you to solve such problems, certain things will be given for example, simpsons 3 8h rule the formula will be given or simpsons one third rule the formula will be given because remembering the formula is not the aim of the course. But to be able to apply that to a given problem is what we aim for. And afterwards we moved away little bit from those kinds of problems we talked about CSTR in little bit more detail.

We told that not only one steady state, but multiple steady states could be available for a particular reactor reactor condition. I mean for a particular inlet temperature and for a particular heat transfer fluid temperature. And so, not only mole balance we needed to do also energy balance in order to get a complete picture of the situation. And we also talked about what we call as ignition temperature and extinction temperature.

So, we plotted the rate of heat removal as a function of reactor temperature or the rate of heat generated as a function of reactor temperature. Because many of these radical polymerizations that you do will be exothermic reactions. So, there will be lot of heat released. So, that heat has to be taken away. So, if you are using these energy balance equations that also gives you an idea, about at what rate you have to take away the heat in order to keep the reactor temperature at a particular value or suppose you want to fix the conversion in this reactor then what is the temperature, at which you have to maintain the reactor in order to get that particular conversion. Those kind of all sorts of variations of problems could be envisaged as far as this thing is concerned. And in detail also we told that the steady state solutions basically they are nothing but the intersection of your RT versus T curve; that is, the rate of heat taken away versus T curve that curve and the curve gt versus T the intersection of these 2 curves.

Gt versus T is basically rate of heat generated versus T. And if you have more than one intersection you are more than one solution basically, then you have more than one steady state. And at each point of intersection the corresponding reactor temperature and corresponding conversion that will define the steady state. So, if you are working at that temperature of the reactor you get that conversion. And given that you have already fixed your inlet temperature and the temperature of the heat transfer fluid. And we are also assuming here for simplicity that the heat capacity of the reactants and products they do not change with temperature so on and so forth.

And then we did some simple problems like all the reaction parameters are given the temperatures are given as far as the inlet temperature, and and the heat transfer fluid temperature constant. Heat transfer characteristics of the reactor are given heat transfer coefficient in the area of heat transfer those things are given. And then we ask you to find out a different steady state operating conditions under this situation. And then we finished up with one simple problem of styrene polymerization where we apply the same concept.

So, I hope that this has given you more or less a holistic view. Probably, we cannot go into much more detail. And we also did not want to stop at a much simplistic version of the reactor problems. So, I wanted to have little bit more a comprehensive overview. So, I hope that it has given you really a good outlook into the into the problem. So, that it can be used as a basis to build further if you are looking for more detailed courses on, basically this is chemical engineering chemical engineering problems. Because this is multidisciplinary field. So, those concepts also are required if you are working in a polymerization plant so on and so forth what not.

So, what we will do is that we will stop the class today. And from tomorrow onwards we go to the last topic of the of the course; that is, we go into the synthesis of different polymers. So, we start with synthesis of different commercially important step growth polymers. And what we will mainly do is to concentrate on the structure property relationship. We would not talk about reactors and how we do the reaction in the reactors in a much more intricate detail no it will be more at the chemistry options, what kind of temperatures we use what kind of pressures we use. And you might think these are some details that are difficult to remember, and you will be right the point is you should remember if you are doing the reaction at high temperature, why you are doing at a high temperature if you have to apply high pressure.

Why you have to apply high pressure, if you are doing a catalysis or if you are splitting up the reaction into 2 steps, what are the pros and cons those are the aspects that we will actually concentrate on not. A specific value of pressure probably you do not need to remember, as long as you know really you are going to go to higher pressure. Or maybe at this stage you have to go to higher temperature, probably you distill up some product that has formed because the reaction is reversible. You want to take the reaction forward. This is one aspect second aspect is more we will concentrate on the chemical structure of this, because it is the structure that gives us an idea about the property that we want to develop unless we understand the relationship between the structure and property we cannot really develop the properties.

So, those are the directions that the course is going to take in the rest of the week, and in the coming week thereafter.

So, until the next class, then goodbye and thank you.