Chemical Reaction Engineering

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Lecture No. # 30

Case Study - Ethane Dehydrogenation

Friends, let us now start looking at reactor design with few examples, that is in the next few sessions we will be looking at some real time reactor design situations, and discussing how we go about designing the reactor. But before we do that it is a good time probably to recap what all things that we have seen so far, so that how we put all these information together to get a meaningful reactor design will become more clear. So, we always started with writing a generalized representation of a reaction, and we did we did this or we rather do this because this allows us to deal with any reaction that we may have.

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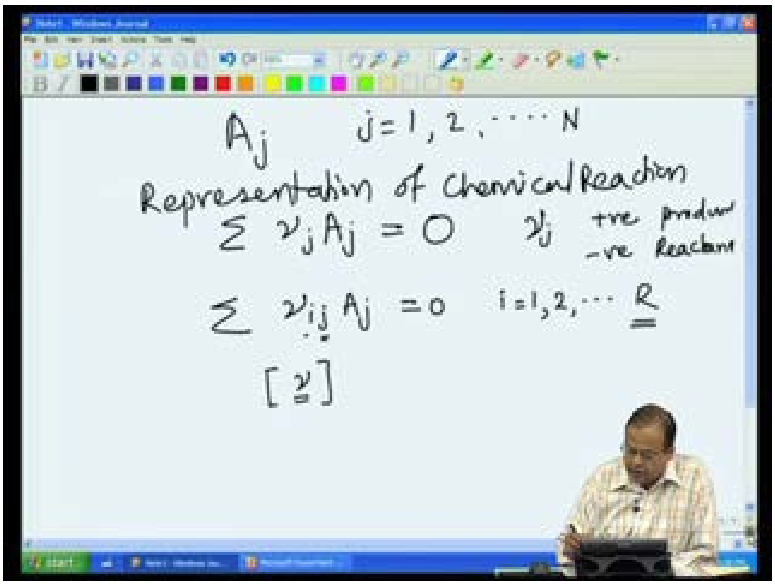

$A_j \quad j = 1, 2, \cdots N$

Representation of Chemical Reaction

$\Sigma \nu_j A_j = 0 \quad \nu_j$ +ve produ
-ve Reactan

$\Sigma \nu_{ij} A_j = 0 \quad i = 1, 2, \cdots \underline{\underline{R}}$

$[\underline{\underline{\nu}}]$

So, leaving the specifics of the reactions aside for time being, we said that we have large numbers of species let us say A j where these species can go from 1, 2 up to some number N. So, we essentially have chemical reactions within this species, and we talked about how we represent this reaction. So that was our starting point, that is representation of chemical reaction. We said that suppose we consider a single reaction, and associate a stoichiometry coefficient mu j with the species A j, then we can write a single reaction are summation mu i j A j equal to 0. By doing, so we are not operary identifying reactions or products by writing them on the left hand side or right hand side of a reaction, but we are doing that by assigning mu j either a positive value - if it is a product or a negative value - if it is a reactant.

Of course when you have a large no of species it is unlikely that there is only one reaction occurring between them. So we extended this representation to consider large no of reactions by seeing that let me associate a subscript i with the reaction. Now and mu i j is the stoichiometry coefficient of the species j in the i th reaction and therefore my i th reaction will be mu i j A j is equal to zero and I can go from 1 to up to R such reactions.

Now why R reactions or what are these R reactions? The reactions that we are interested and that we will focus while representing this generalized form are only independent reactions. So we do not want a reaction and the same reaction represented by multiplying the stratum all the stoichiometry coefficient by a constant number except zero to be part of our reactions scheme as two separate reactions. So we eliminate all those and how we do that we look at the rank of the matrix stoichiometry matrix nu bar and that rank tells me how many independent reactions are in my system.

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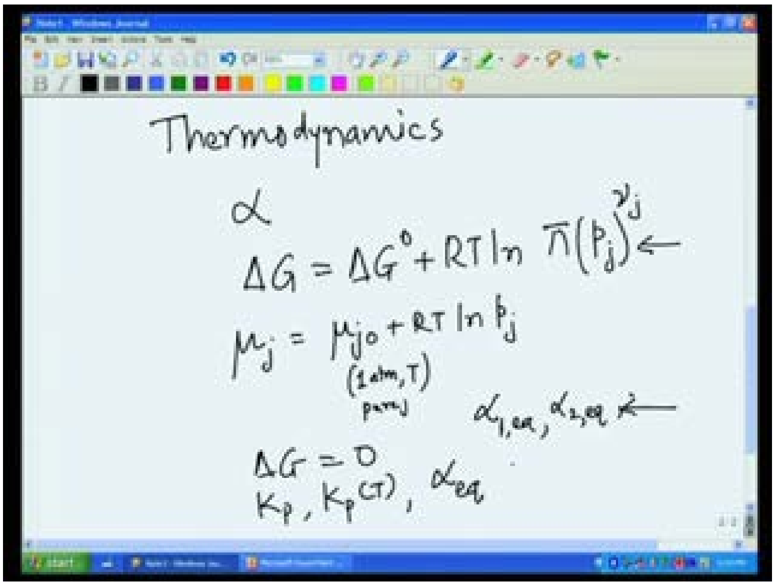

Thermodynamics

α

$$\Delta G = \Delta G^0 + RT \ln \prod (p_j)^{\nu_j} \leftarrow$$

$$\mu_j = \mu_{j0} + RT \ln p_j$$

(1 atm, T)
pure j

$\alpha_{1,eq}, \alpha_{2,eq} \leftarrow$

$$\Delta G = 0$$

$K_p, K_p(T), \alpha_{eq}$

So this was about how we represented the reactions then we spend little bit of time on looking at thermodynamics of the reaction. Now why is thermodynamics important? It is important because it gives us what are the achievable conversions or limit to how we can us how much reaction will progress. How do we measure the progress of a reaction we defined variable alpha as extend of a reactions and then try to see what will be the limit on these extend of reactions, when we have a chemical reactions such as mu j A j is equal to zero and this lead us to using free energy concept.

And seeing that delta G the free energy change is delta G zero plus RT l n product of let say if we are writing a gas phase reaction of ideal mixture behavior p j race to race to mu j and to arrive at this equation. We took help of chemical potential mu related for the species j to a let say in an ideal gas mixture. The standard condition chemical potential what are the standard conditions reference pressure is usually one atmosphere the temperature T of the mixture and pure j as the component. Now thermodynamic tells us that reaction will occur if free energy changed is negative and moments free energy change becomes zero we have an equilibrium reaction.

So equilibrium of a reaction then it is characterized by delta G is equal to zero and from this point onward we defined the equilibrium constant k p how it depends on the properties for example, k p T then using this p j partial pressure in terms of mole fraction into total pressure bringing in the stoichiometry mass balances. We found out how we can find equilibrium extend of extend of reaction.

If there are large number of reactions no problem we have equilibrium extend of reaction for one, for reaction two, reaction three and so on and thermodynamic tells us that if there are R reactions than at equilibrium all individually each of these reactions is at equilibrium. So we have R such conditions which allow us to calculate R unknown values of alpha.

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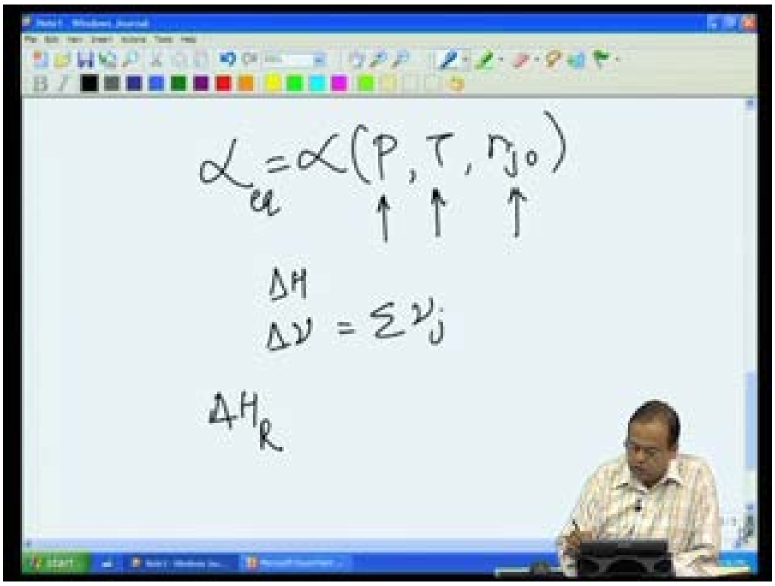

$$\alpha_{eq} = \alpha(\underset{\uparrow}{P}, \underset{\uparrow}{T}, \underset{\uparrow}{n_{j0}})$$

$$\Delta H$$

$$\Delta \nu = \Sigma \nu_j$$

$$\Delta H_R$$

We also saw how these alpha changes for example, how this alpha is dependent on the pressure of the system is dependent on the heat of reaction or rather how it is dependent on temperature, how it is dependent on the initial moles of the system and so on. So the idea was that we have alpha equilibrium and how can we change these equilibrium value of alpha because if it is a reversible reaction alpha is some finite value. Now if we want to increase this equilibrium conversion so that we can realistically get higher conversions in our reactors.

Then we have to play around with the operating condition such as pressure, such as temperature the composition of the system and so on and this largely depends on the heat of reaction so temperature effect for example, is related to what happens if the reaction is exothermic the equilibrium conversion decreases as temperature increases and so on. It also depends for gaseous reaction for example, on change in number of moles, which is summation mu j and that allows us to determine; what we should do with pressure should we have low pressure reaction high pressure reactions and so on. Thermodynamic also tells us about the heat of reaction and how it changes with temperature.

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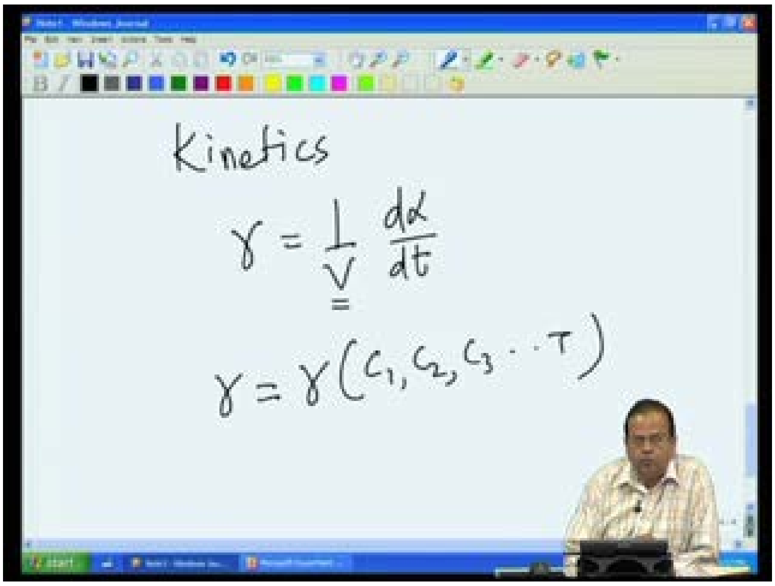

Kinetics

$$\gamma = \frac{1}{\underline{\underline{V}}} \frac{d\alpha}{dt}$$

$$\gamma = \gamma(C_1, C_2, C_3 \cdot \cdot T)$$

So armed with all these information we than focused our attention on the kinetics of the kinetics of the reactions; kinetics that is the measure of rate of reaction and these rate of reaction, we define for a close systems as how the what is the rate of change of extend of reaction with time. And it define it as intrinsic variable as a normalizing it with the volume of the reacting mixture depending on whether the reaction is homogeneous or heterogeneous. We can have different normalizing factor such as volume of the reacting mixture or the weight of the catalyst and so on.

We are also then interested in what are the factors which influence this rate of reactions. So for example, concentration temperature and so on and we saw few basic kinetic such as law of mass action kinetics power law kinetics of edge first order reaction for example, is one of the specific case of power law kinetics.

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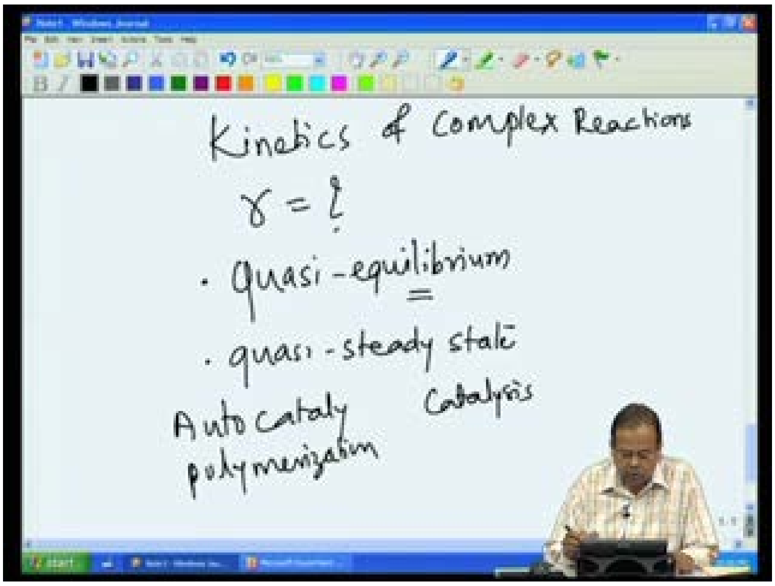

Kinetics of Complex Reactions

$r = ?$

- quasi-equilibrium
- quasi-steady state

Auto cataly

Catalysis

polymerization

We then turned our attention to kinetics of complex reactions. Because in real life the reactions are hardly display hardly ever simple behavior or reactions are complex and there are several reasons why reactions can be complex. For example, there can be large number of reactions and reactants. There can be number of steps through which reactions proceeds before we get our desired product and all these contribute to kinetics and reactions being complex. Now to deal with complex reaction kinetics and get what is the r or rate of these reactions.

We essentially develop two concepts namely quasi equilibrium approximation where we say that if there is large number of reactions then one or more than one are the rate determining steps and all other reactions are the slow reactions and all other reactions have attend their equilibrium. So we have idea of equilibrium but not for the entire reacting system because if the entire reactions systems of attends equilibrium our rate is zero. So quasi equilibrium so there are certain reactions which are slow so compared to this reaction all other reactions have reached equilibrium and that is quasi equilibrium approximation.

The other idea is quasi steady state and here we apply this idea to species rather than to the reactions. So we say that dynamic of certain species is slow compared to other. So those species which are highly reactive or whose dynamics is very fast they attend their steady state much fasters before the slow species can show any progress measurable progress. So we apply steady state but if again if we apply steady state to all the species then net rate will be zero.

So we apply steady state to few species, which are highly reactive and then use what we call quasi steady state approximation to attend the rate of rate of reaction and we illustrated this concept by taking few example for auto catalytic reactions or polymerization reactions, catalysis reactions and free radical mechanism reactions and so on. So we then saw how we determine the kinetics of the reactions.

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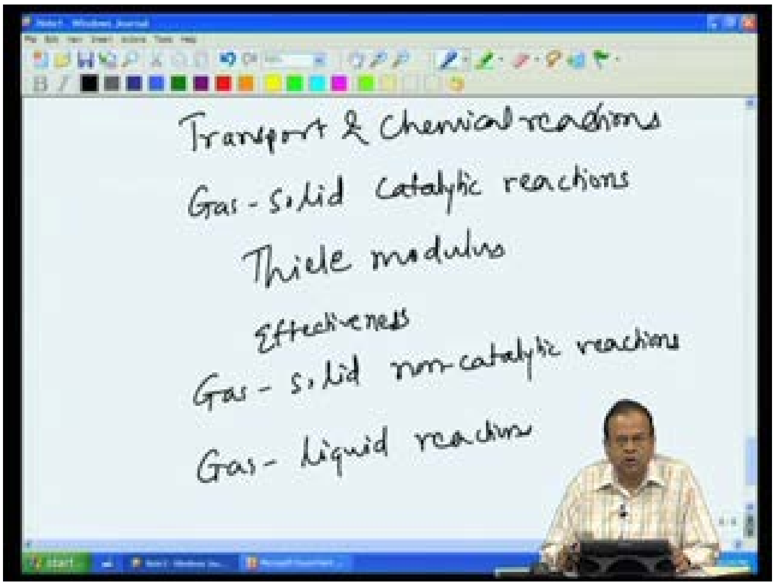

Transport & Chemical reactions

Gas - Solid Catalytic reactions

Thiele modulus

Effectiveness

Gas - Solid non-catalytic reactions

Gas - Liquid reactions

We then turned our attention to looking at what happens in the reaction when we have more than one phase present in the system namely heterogeneous reactions. So we focused for example, so we looked at transport phenomena and how it influences the chemical reactions. And for these we looked at two different kind of three or two or three different processes. First was a gas-solid catalytic reaction. So here we saw first of all what is happening when gas-solid catalytic reactions are taking place that is what are the various steps that gases molecules has to undergo before reaction can take place. So the catalytic component is on the solid the reactants and products are in gas phase.

So there has to be diffusion from bulk to the surface from surface to the inside of the catalyst for the reactant than the reaction and then diffusion of the product in the brewers direction. So as a result of presents of all these mass transport or diffusion processes the kinetics of the process is not just the kinetics of the chemical reaction or the intrinsic kinetics it can get massed with the transport behavior and therefore, we defined how we can how we can combine this two and see what is the effect for example, how do we measure whether mass transfer is limiting or not. So we have for example, Thiele modules then we have concept of effectiveness factor and so on.

We also applied similar ideas to gas-solid non-catalytic reaction, where we said that things like diffusion are still the same except. Now the solid is not static that is it is undergoing a change. It is undergoing a change in form of its shape either particles are dissolving or something is getting deposited and so on. So it becomes a dynamic process so to that extend it is different and catalytic reactions but certain aspects such as diffusion and whether mass transfer controls or chemical reaction control remain the same. We also then looked at gas-liquid reactions and idea such as enhancement factor effectiveness factor and so on.

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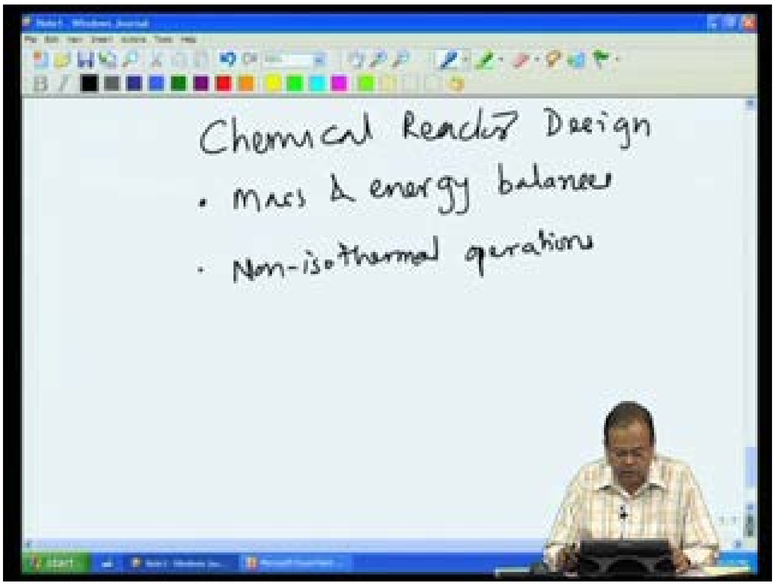

Chemical Reactor Design

- Mass & energy balances
- Non-isothermal operations

So we started with kinetic we then brought in transport and then we wanted to put all this things together. So we started looking at chemical reactor design and for this what we are currently discussing, we initially started with looking at mass and energy balances. Then we looked at what happens when we have non isothermal operations. Why these are important, adiabatic reactors, isothermal reactors or combination there of so having now acquainted ourselves with all these information.

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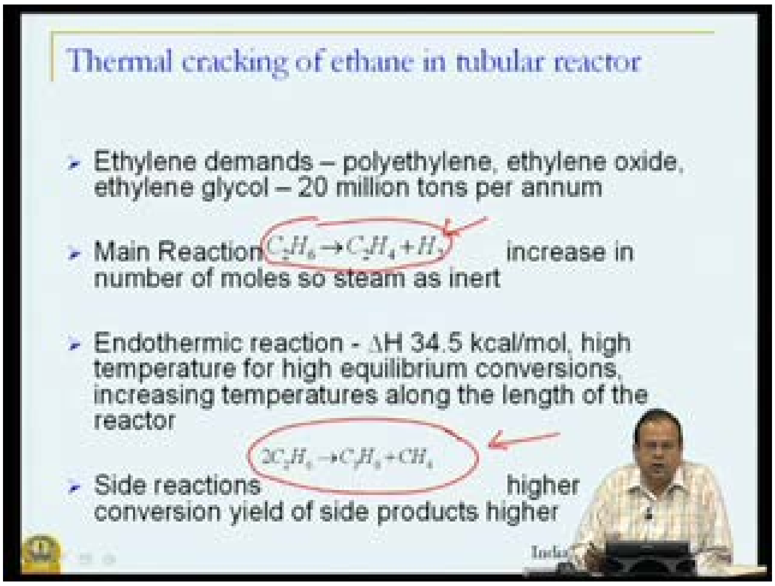

Thermal cracking of ethane in tubular reactor

- Ethylene demands – polyethylene, ethylene oxide, ethylene glycol – 20 million tons per annum
- Main Reaction $C_2H_6 \rightarrow C_2H_4 + H_2$ increase in number of moles so steam as inert
- Endothermic reaction - ΔH 34.5 kcal/mol, high temperature for high equilibrium conversions, increasing temperatures along the length of the reactor
- Side reactions $2C_2H_6 \rightarrow C_3H_8 + CH_4$ higher conversion yield of side products higher

Let us try to put all this information into practice by looking at various reactor design case studies and the first case study that we are going to look at is that of thermal cracking of ethane in a tubular reactor. Now all we need to crack ethane for example, after it is cracking use ethylene and I do not think I need to expand on why we need ethylene. We need polyethylene, ethylene oxide, ethylene glycol and most of other product for which ethylene is a starting material and at one estimate the production of ethylene exceeds some things like twenty million tons per annum.

This slightly old information may be around two thousand; four or five this was the number I could get my hands on may be the demand has increased further. So what is the main reaction here? So the main reaction for this is the cracking of ethane so ethane molecule C 2 H 6 gives ethylene C 2 H 4 and another molecule of hydrogen. Now if you look at this reaction clearly starting with one reactant mole, we get two moles of product so there is a increasing in number of number of moles and it is a gaseous reaction.

So increasing numbers of moles for example, if you want to achieve high equilibrium conversions; one of the things that you can do is actually increase the total number of moles initially present by adding some inerts and in this particular case we add steam for it. So we have steam added although steam does not participate in the reaction. We add it as an inert to achieve higher equilibrium conversions. So endothermic reactions and the heat of reaction is plus 34.5 kilo calories per mole fairly reasonably high value, since it is a endothermic reaction if you carried out an equilibrium look at the equilibrium of these reactions higher temperatures for higher equilibrium conversions.

Now if we have a for example, we saw how to operate such reactors in a batch reactor, we would have to progressively increase the increase the temperature as function of time or in the tubular reactor that would translate into increasing temperatures along the length of the reactor. Even if you do not want to increase the temperature because this reaction is endothermic what we will get is as reaction takes place and if you are not trying to control the temperature; there will be natural tendency for temperature to go down because it will reaction will take away energy from the system.

So, even otherwise we will have to somehow keep heating this system to maintain the isothermal temperature and if you want to achieve these increasing temperature profiles along the length of the reactor, we will have to adopt some novel strategy. So that the temperatures not only remains same constant but keep increasing along the length of the reactor. Another aspect of this reaction is that this is cracking or this is not the only reaction that takes place. In fact there are several side reactions which are possible and this side reaction shown one shown over here is two ethane molecules combining to give us a butane molecule and a methane molecule and there are several such side reactions. But the point is that these reactions dominate at higher conversions.

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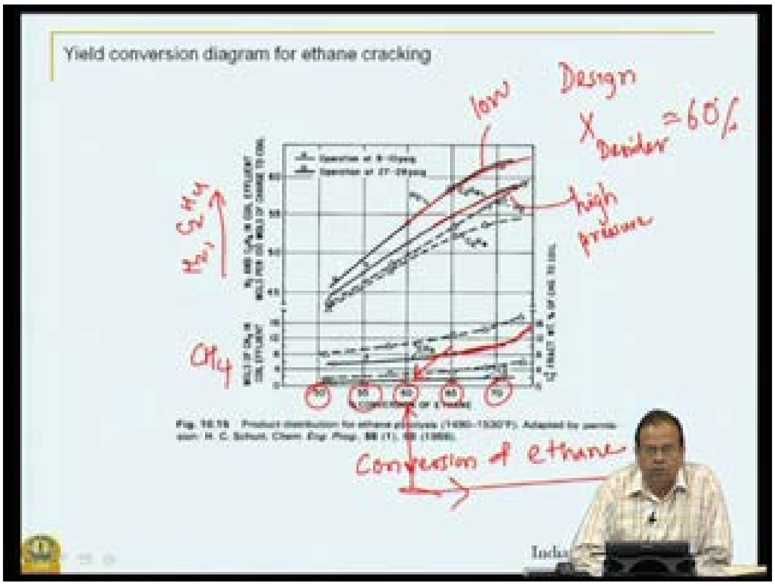

Yield conversion diagram for ethane cracking

So as our conversion increases and the side product also go on increasing and this is shown in what we had earlier before two as the yield verses conversions conversion diagram; so what we have here is on the x axis is conversion of ethane on the x-axis and on y-axis we have this one is H 2 and ethylene moles per mole hundred moles of hundred moles of ethane. So we have that and on the bottom is the methane I discussed that is one of the one of the side products in the reactions. So what we see here is as conversion is increasing from example from fifty percent from to fifty five to sixty the moles of ethane and ethylene are increasing, moles of ethane and ethylene are increasing.

But what we see is that as the conversion increase to sixty five or seventy percent there is much more rapid increase in the methane that comes out compared to the ethylene. For example, if you look at hydrogen or ethylene it is started saturating and more and more of ethane or bio product is coming into the system. What it implies is that two things one is you do not want high quantity of methane. So it implies that you have to stop your reaction at around sixty percent conversion. So what it implies is that you have to stop this reaction at sixty percent sixty percent conversion.

That means even though you have a possibility of converting hundred percent ethane. Now remember this is a multiple reaction so hundred percent conversion of ethane does not mean equivalent amount of ethylene being formed. In fact that this study studies shows you will get at higher conversions more and more methane. So the design objective for example, here that is x or conversion desired is not hundred percent but roughly sixty percent or 0.6 so that is that is one aspect. The second aspect that is also apparent here we see the results at two different pressures, this is let me just say low pressure and this is high pressure.

Now why is this happening because there is an increasing numbers of moles lower pressure will favor higher equilibrium conversions? So typically the operating pressures are on the lower side but then there is also another limit you cannot have very low pressure. For example, can you do this reaction under vacuum? Just for sake of argument no because under low pressures for gaseous reaction also means low concentrations and which means low rates of reaction; so one has to strike a balance between again getting higher pressure higher rates of reactions and higher equilibrium conversions. So pressure is also an important factor.

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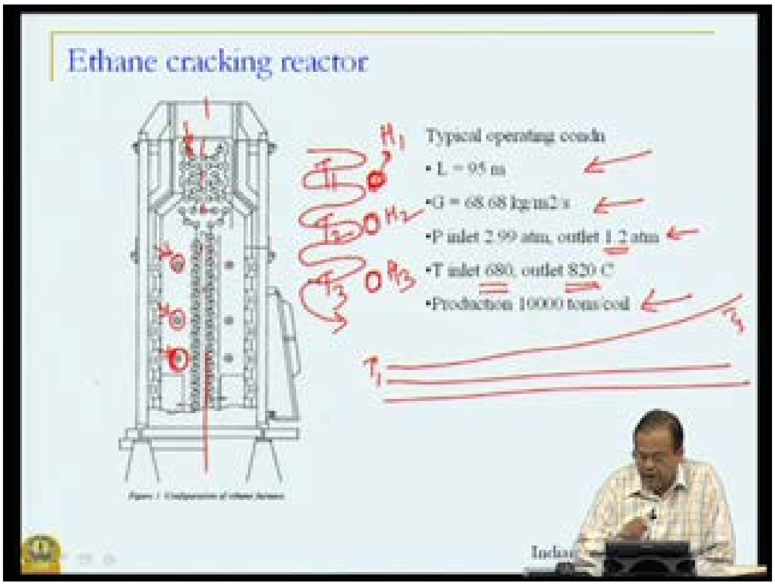

Ethane cracking reactor

Typical operating condn

- L = 95 m
- G = 68.68 kg/m2/s
- P inlet 2.99 atm, outlet 1.2 atm
- T inlet 680, outlet 820 C
- Production 10000 tons/coil

Given all these typical operating conditions for ethane cracking reactor, which is shown over here ethane furnish as it is called I will explain what this furnish is but typical conditions are length is 95 meters. The gaseous flow rate or the flux is about 70 kilogram per meter square per second inlet pressure is about three atmospheres outlet pressure is about 1.2 atmosphere and we will come back to this factor when we talk about design of this reactor. The inlet temperature is 680 and outlet factor is 820. So it is progressively increased and one cube and I will explain what that cube is gives you about ten thousand tons per tons per coil.

Now how is these reactor fabricated now when you say that length is 95 meters; one way of thinking that is a horizontal tube or a vertical tube horizontal is what comes to mind immediately of the entire length occupying 95 meters. Now that will take too much of a space and the world where space has a premium you do not want that so what do you do you do not go horizontal you go vertical and this is precisely what is done in this reactor; so let us look at what this reactor is. First of all there is an actual cemetery and so you have roughly the same things happening on the both side of the reactor and how this reactor design there is is an inlet at this point and then the tubes are actually coiled.

So if you look at the look at the cross section it would look something like this. So it is not a straight tube but a coiled tube with the outlet coming out over here. So if you look at the side view this is what this is what you will see. So this is how the entire length of the reactor is reactor is achieved. So instead of having long single long tube you have a coiled tube and it is a same things on both sides. Now you also want fairly high temperatures. So how do we achieve that so for that what we have on the sides what you see here are actually flue gas burners and therefore, these are what are called as furnaces.

So you are actually burning flue gases or passing flue gases hot flue gases through the external of this of this coils there by achieving two things. One achieving high temperature and by controlling the flux heat flux of each of this burner. You are now are in a position to achieve different temperatures along the length of the reactor why is that for example, if you again look at the side view what you are seeing is that in this regime the heat flux will be let us say some H 1, in this regime it will be H 2. So again these are the burners that you are seeing here H 3 and so on.

So we can have temperature T 1 in this regime temperature T 2 in this regime temperature T 3 here and so on. So essentially we have therefore, generated a profile of temperature along the length of the reactor. For example, if I say this is my low temperature to a high temperature. Now how do we achieve exactly how how we can module does this at this point let us not worry about how it is achieved? I will come to the module of these reactors itself and then I will just mention how we can add to this to this module.

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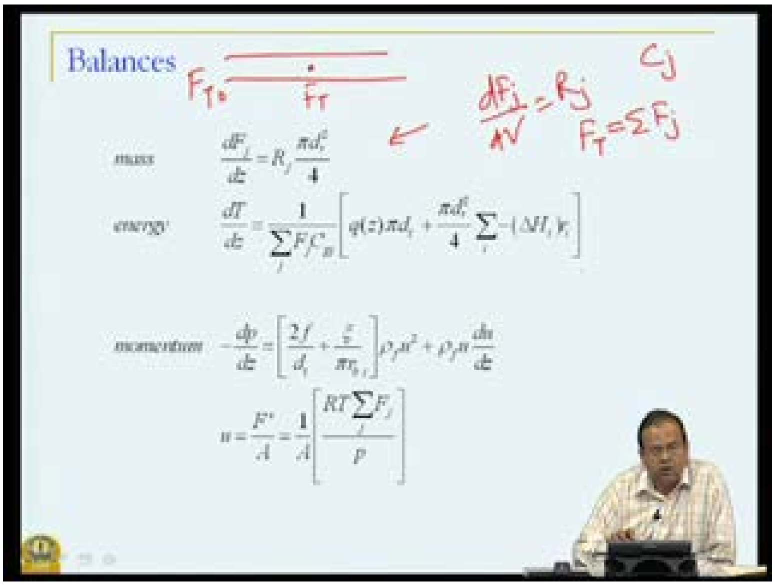

Balances

F_{T0} $\dot{F}_T$

$\frac{dF_j}{dV} = R_j$ C_j

$F_T = \Sigma F_j$

mass $\frac{dF_j}{dz} = R_j \frac{\pi d_t^2}{4}$

energy $\frac{dT}{dz} = \frac{1}{\sum_j F_j C_{pj}} \left[q(z) \pi d_t + \frac{\pi d_t^2}{4} \sum_i (-\Delta H_i) r_i \right]$

momentum $-\frac{dp}{dz} = \left[\frac{2f}{d_t} + \frac{\zeta}{\pi r_{b,t}} \right] \rho_f u^2 + \rho_f u \frac{du}{dz}$

$u = \frac{F'}{A} = \frac{1}{A} \left[\frac{RT \sum_j F_j}{p} \right]$

So these are our balances which we use for design of this design of these reactors. What are these what are these balances? These are our simple mass and energy balance and a momentum balances balance as well. Now what is this mass balance this mass balance is actually the same things as dF j dV is equal to Rr j that we had seen we are assuming only a tubular reactor. Now where we dealing with F j and not concentration C j, the reason being if you recall when we talk about stoichiometry tables we have increasing numbers of moles; so F total for example, at any point of time that is suppose you take it as a as a reactor and total moles that are entering if F t zero at any point of time is F t then these F t is not same as F t zero. So there is change in numbers of moles which results in change in either the volumetric flow rate or change in concentration and so on. So we deal with dF j dV which translate into this equal to equal to R j.

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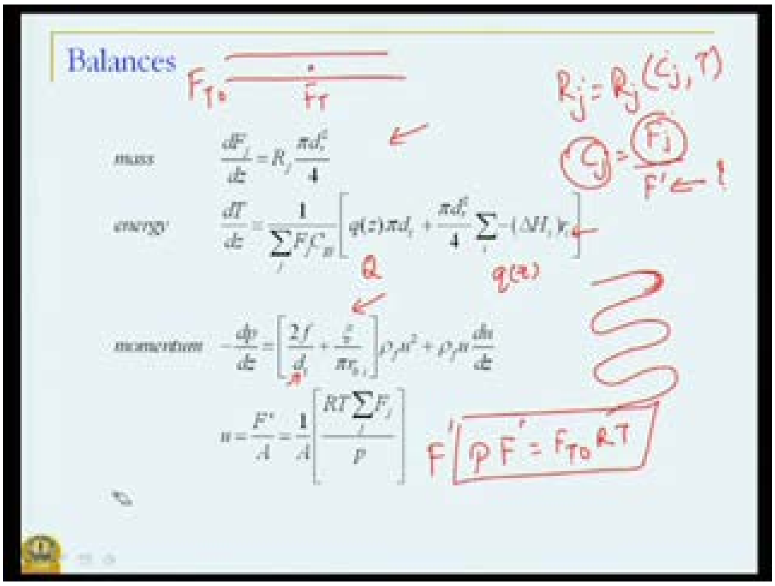

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Q

q(z)

momentum $-\frac{dp}{dz} = \left[\frac{2f}{d_t} + \frac{\zeta}{\pi r_{b}}\right]\rho_g u^2 + \rho_g u \frac{du}{dz}$

$u = \frac{F'}{A} = \frac{1}{A}\left[\frac{RT\sum_j F_j}{p}\right]$

$R_j = R_j(C_j, T)$

$C_j = \frac{F_j}{F'} \leftarrow ?$

F' $\boxed{pF' = F_{T0}RT}$

Now what is R j? R j is a function of concentration that is a reaction rate for the j th species for first of all what are j th species. We list out all these species that are there for example, ethane ethylene hydrogen butane methane and so on. So those are the species R j is a rate of change of species j in all the reactions and these is a function of concentration temperature and so on. What is concentration is F j by the volumetric flow rate v or F prime. I use the symbol F prime so let us stick with that so this is nothing but F j by F prime concentration. So we have mass balance equations in terms of F j we have rate which is in terms of concentration. So we have to find out figure out what these F prime F prime is.

Second is the energy balance. Energy balance also is the same as the energy balance for a tubular reactor except the term Q that was that was there that is the heat added to the system is now represented in terms of the flux Q j q q of z; that is what is the heat flux of those burners side various different locations and since it is changing along the length of the reactor we represent it as q of q of z and of course, the contribution second term here in the energy balance represents the contribution due to all the reactions. So that is my energy balance. So I do not have isothermal reactor neither do I have an adiabatic reactor but I am somehow going to achieve some temperature variation through use of these burners.

Now if you remember the configuration that we talked about this is actually a reactor tube tubular reactor with lot of bends and a long length or reactor. So these in this you can you can easily expect that there will be some pressure drop and that is a reason we have to account for these pressure drop. Now why do we have to account for this pressure drop now why do we have to account for this pressure drop will become clear in just a minute. So what we have is the momentum balance which accounts for these for this pressure drop this term is familiar friction factor terms and this is to account for the bend the pressure drop across the bent. So zeta is chief factor pi r b i so r b i for example, radius for this bend and so on.

So we have now our momentum transfer and momentum transfer has velocity u for example, which is the flow rate F prime by A and now how do we get our flow rate F prime. We use our ideal gas flow for example, if we assume this ideal gas law then the total pressure into F prime is F T zero RT. A version of an ideal gas law for a flow reactor where instead of volume you have volumetric flow rate instead moles you have the molar flow rate. Now my F prime is RT summation F j which is which is F T zero divided by the pressure p and now this forms my complete module but it is interest in to see how different things are related to each other and we will we will just look at the coupling between mass momentum and energy balance.

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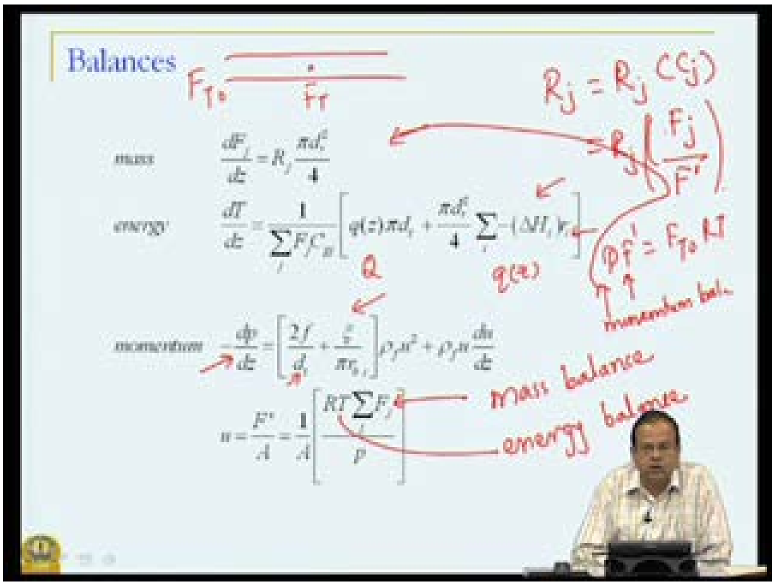

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Let us start with the momentum balance. So one should think that why the momentum gets influence by how the mass is changing in the reactor. But when we have the chemical reaction with change in numbers of moles they are indeed connected now how. We look at this pressure balance or the momentum balance where these terms tell us how pressure is changing along the length of the reactor and this has velocity terms and density term and so on. Now what is a velocity, now if you look at is RT summation F j by p. F j coming from mass balance equation, temperature coming from energy balance equation. So our momentum balance equation is coupled to mass and energy balance equation.

Now what about mass and energy balance? Of course, they are they are related to related to each other why because we said that R j look at the mass balance. R j is a function of concentration is nothing but the molar flow rate divided by F prime. Now F prime is given by u into a for example, and we see here that as for example, what is F prime p F prime is F T zero RT. So F prime changes as pressure changes. So this is my momentum balance term. So this is now linked to mass balance equation because of it is appearance in the R j terms and of course, we have already seen mass and energy balances are related because of same rate of reaction is depended on temperature.

So we have mass momentum energy balances completely linked to each other. We can of course, do the same exercise as energy balances and I leave it to for you to figure it out or in other words when we have such a reactions in a reactor; there is a strong coupling between mass energy and momentum balances and these is a reason why you would see that the inlet; for example, pressure is 2.99 inlet pressure three atmosphere outlet is only about 1.2, almost fifty percent or little more than fifty percent pressure drop.

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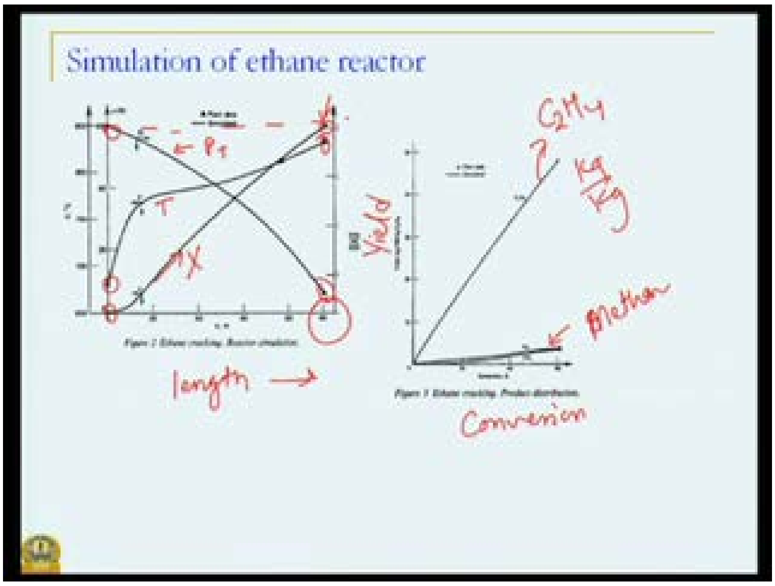

Simulation of ethane reactor

So how does for example, when you put all these things together this is a typical simulation of ethane reactors. So what we have here is the length of the reactor ninety-five typically ninety-five. We have conversion x then we have temperature along the length of the reactor and we have total pressure p T and what do we see conversion of course, increases as time or as along the length of the reactor. Remember we are talking about the tubular reactor here; so conversion increases as we travel along the length and how it is influence by for example, pressure which is decreasing and temperature which purposely we had we had modeled our furnaces or the fluxes heat transfer fluxes such that we get higher temperature or increasing temperature along the length of the reactor.

And what we see here is the points although you do not see those these are the typical inlet outlet conditions and it is a fairly good match between the model simulations. For example, this will tell me that if I want to conduct my reaction up to sixty percent conversion I have to have my reactor which is about ninety-five meters long and in fact that that is the reactors lens that are that are used. And on the on the side here is again yield conversion diagram for the industrial reactor. So we have yield of yield of ethylene over here and yield of ethane sorry methane and hydrogen.

Now remember this is expressing in terms of kg per kg and in terms of moles the molar yield ethylene and hydrogen should have ethylene and hydrogen should have been same. But in terms of mass they are they are of course, of course, different hydrogen being much lighter than or lighter than ethylene. So this is as far as the design of ethylene reactor is reactor is concern. So what we what we saw here is basically a homogeneous reaction. So not much to be a expected in terms of transport and all that but still transport is indeed the important.

Because if you look this simulation for example, if we had assumed constant pressure constant pressure, you can imagine how much results would have been off because your pressure is actually decreasing by more than more than fifty percent. So this example for illustrates how do we use thermodynamic information because there is increasing number of number of moles we have to have low pressures inerts to achieve higher equilibrium conversions. We also we also saw that say endothermic reactions so increasing temperature profiles is desirable.

So how thermodynamic information is brought in kinetics of course, is of course, is important so ethane carting for example, thermal cracking is a free radical reactions so it has been modeled accordingly so on and then bringing the mass energy and momentum balances together to achieve the achieve the desired objective. Now I have mention that in this model we just assume that we are going to program our furnish to achieve this heat flux balances. So what we are saying is suppose this is my tube in which ethane is flowing and this is my shell and I am just saying that there will be heat transfer from here to here which is Q object.

Now if I want to make this model more realistic why do I bother about bother about few objects? I can express it in terms of temperature of these flue gases that I am passing through. So I can bring in the reference or T r temperature which again will change along the length of the reactor. But this Q object then related to temperature difference between the inside the tube and outside the tube or other way out T r minus T. So we can add one more balance for how T r changes along the length of the reactor.

Now that will depend on what is the burning rate of the flue gases or the burning efficiency of the flue gases and so on. So we can actually go on the expanding the model in terms of the details that we want but what we saw here was a base level model where we say that we just assume that there is certain heat flux that we can achieve and that changes along the length of the length of the reactor. So this was our first case study.

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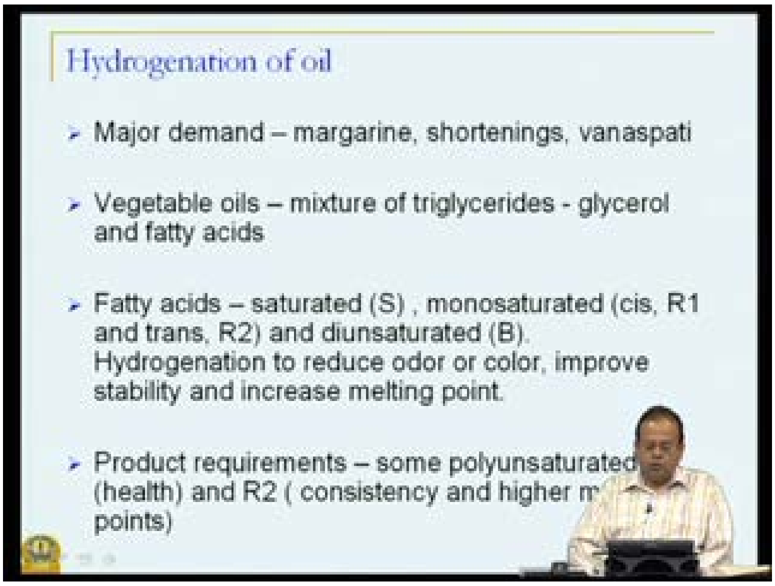

Hydrogenation of oil

- Major demand – margarine, shortenings, vanaspati
- Vegetable oils – mixture of triglycerides - glycerol and fatty acids
- Fatty acids – saturated (S) , monosaturated (cis, R1 and trans, R2) and diunsaturated (B). Hydrogenation to reduce odor or color, improve stability and increase melting point.
- Product requirements – some polyunsaturated (health) and R2 (consistency and higher m points)

Now let us turn our turn our attention to second case study and I will just have a brief introduction in this session and we look at the kinetics in the next class and this example is an example of a design of a batch reactor for hydrogenation of oil. Now why do we need to hydrogenate oil? There are several reasons why oils are hydrogenated and their major demand for example, is in hydrogenated oil or what we called dalda or vanaspati or various different brand names.

But basically it is for using it oil as margarine or shortening that is substitute for butter or shortening and so on as a cooking medium. Now what is wrong with using oil itself? Of course you can use oil but as you know oil at room temperature is liquid and to transport for example, this liquid is a major problem; so one of the reasons while we can hydrogenate because hydrogenated oils are in the solid form. So if you want to transport them that are much more much more easier. So what happens when you hydrogenate oil?

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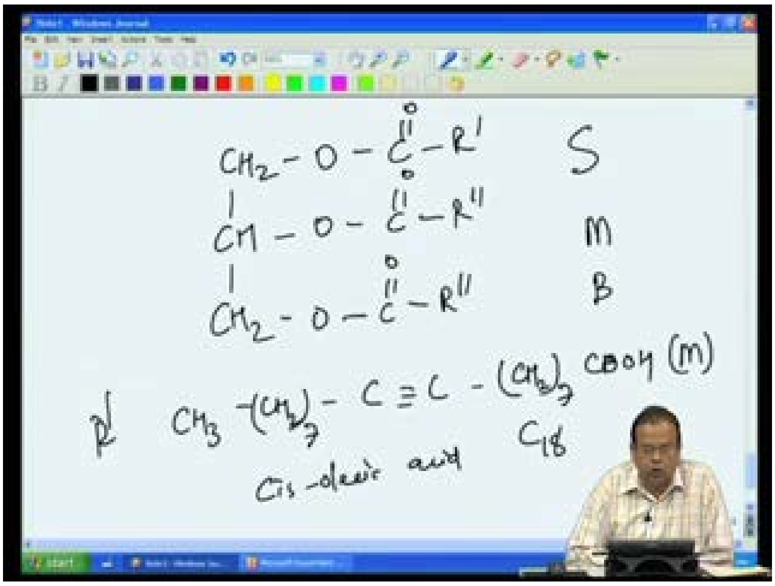

Now, what happens is the following. So let us see what is oil? As you know oils for example, if you take cotton seed oil or any such oil, it is actually a tri glycerite. So, it is a mixture of or it is an ester of glycerol whose basic back bone is this. So, if you had OH OH OH we have glycerol, but it is a it is a ester. So we have an acetic or we have an acid. So the basic hydrolysis reaction for example, if you hydrolyze this you get CH 2 OH CH OH CH 2 OH, and so on. Now, this try glycerite as you know we are also looking at as a source of biotic cell, and that is where clash arises do we use it as a food or do we use it as a as a fuel.

But let us we keep aside that conflict for the time being let us focus on the reactor design. So what are what this different fatty acid is? For example, these fatty acid are long chain long chain aliphatic acid. So what essentially we have for example, if you have something like oleic acids cis-oleic acids it is so that is my cis-oleic acid. So long change so total number of carbon is 1 2 7 8 7 8 9 10 17 18 C 18 and there are various versions of this for example, we could have a single double bond. So what we call mono unsaturated acid or a triple bond a triple bond where which is linolenic acid. So I will just rub out this and say die unsaturated fatty acids and so on.

So we have saturated fatty acids where there is no double bond so when you hydrogenate this oil essentially what you are doing is you are adding hydrogen in the R prime group. So this is my R prime so in the R prime. So we have the let us say di unsaturated then we have mono unsaturated and then we have saturates. Now why do we why do we hydrogenate? As I said it changes the density. It also makes it more stable by increasing the melting point so essentially we have solid.

Also does another thing it reduces the order and changes the color to a pleasant color. So we can actually get it as a pleasant edible matter; if you are using merger into spread on to your butter roll one something which is a pungent order or something which is not appetizing so to speed. So we do it for changing the order we do for changing the stability. So what is where is the where the design here is? Now what happens is that if you hydrogenate and you started getting or going from di to mono to saturates.

Now you may say that I will saturate so that all there are no double bond or triple bonds at all. Now it turns out from the prospective it is desirable to have certain mono unsaturated in your in your oil. So you do not want to saturate them completely yet you do not want to lose them di unsaturated as well because that will make them make them in the liquid form and so on.

So, in the next session, we will see how do we how do we design reactors for this. Now I will just mention at this point what we have here is a liquid, then we are going to say we are going to have hydrogen, so gas and to add more complexity this requires a catalyst. So, we have solid liquid gaseous reacting system. So, we will see this as an example of a design of a slurry reactor if you like to call, slurry here that slurry being of the catalyst. So, that will be the topic of discussion for our next session. Thank you.