Chemical Reaction Engineering

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Lecture No. # 27

Chemical Reactor Design: Mass and Energy Balances

Friends, let us continue our discussion on gas-liquid reactions, and in this session we will wrap up that discussion and start looking at reactor design. Now, last time we saw few cases depending on whether the reaction is slow or fast or moderately fast, how reaction is likely to proceed. That is if the reaction is extremely slow, and if we are looking at gas-liquid reactions in the framework of two film theory, then there is hardly any reaction in the hydrodynamic or mass transfer boundary layer, and the entire reaction is restricted to the bulk.

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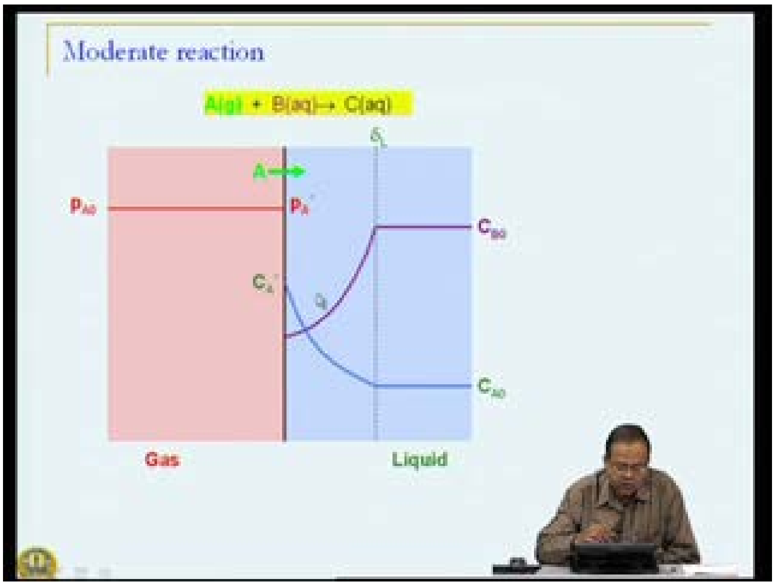

Moderate reaction

$A(g) + B(aq) \rightarrow C(aq)$

Making reaction little faster gives you a picture, which looks something like this that you have a hydrodynamic boundary layer in which there is diffusion and reaction, which is simultaneously taking place. Apart from the fact that there will be a reaction in the bulk liquid, and when we deal with these kinds of reactions, there are two ways of looking at these reactions namely rating by looking at what is the observed rate, and what would have been the rate if mass transfer limitations were not there. That is a traditional way, which we saw even for gas-solid catalytic reaction.

But another way of looking at the same process is what is the observed rate and what would have been the rate if reaction was not there. That means we are looking at absorption of gas A from the gaseous phase into the liquid. So what would have been that rate if only mass transfer was there that is there was no chemical reaction and we saw that because of chemical reaction there is actually enhancement of the observed rate. That is the mass transfer with chemical reaction results into rate of higher rate of absorption of gas into the liquid.

If that is the case then in designing any gas purification streams one would like to have as high reaction rate as possible. Because that would enhance the absorption of gas to the maximum extent possible and therefore, we have reactive species in the liquid when we try to absorb any gas even though gas may have some partial solubility in just water. But that would be simply case of mass transfer and when you add a reactive species like potassium hydroxide or sodium hydroxide or ethanol amines, then you are actually making the aqueous solution reactive, so that there is mass transfer with chemical reaction.

And since we are also looking at increasing the rates of reaction then we are also looking at increasing the temperatures for example, hot solutions so that reaction rates are higher. Now we need to now start worrying about, what will happen if the reaction rate is even faster? So we have a fast reaction, which case as you can see from here our concentrations of these two species in the bulk will start going down. That is if the reaction in this hydrodynamic boundary layer is faster and faster then the concentrations of A and will go on depleting faster and faster.

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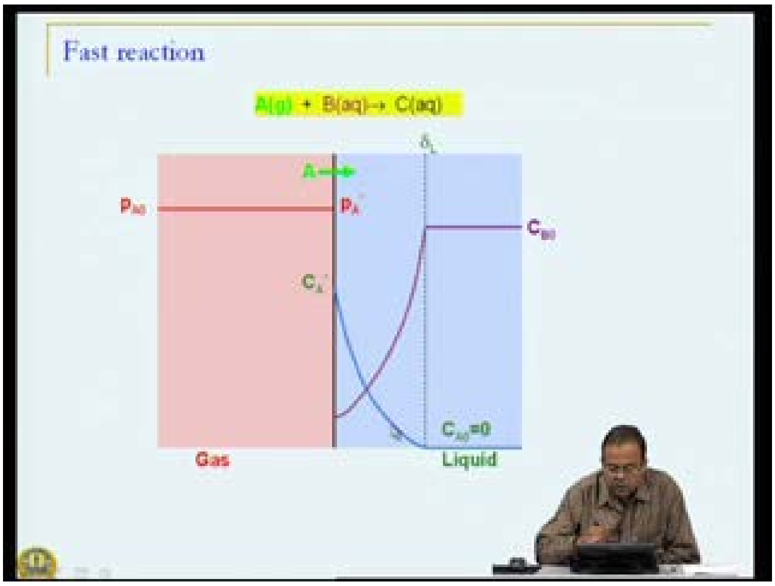

Fast reaction

$A(g) + B(aq) \rightarrow C(aq)$

And we may come across a situation for moderately fast to fast reaction, where by the time A reaches the boundary layer thickness delta L entire A is consumed. If that is the case then there cannot be any reaction in the bulk but the reaction would be limited only to the hydrodynamic boundary layer that is what will happen if the reaction is fast. Let us make reaction even faster because we saw that there is order of magnitude difference in kinetic rate constants of different reactions gas-liquid reactions. So what will happen if we make it even more faster?

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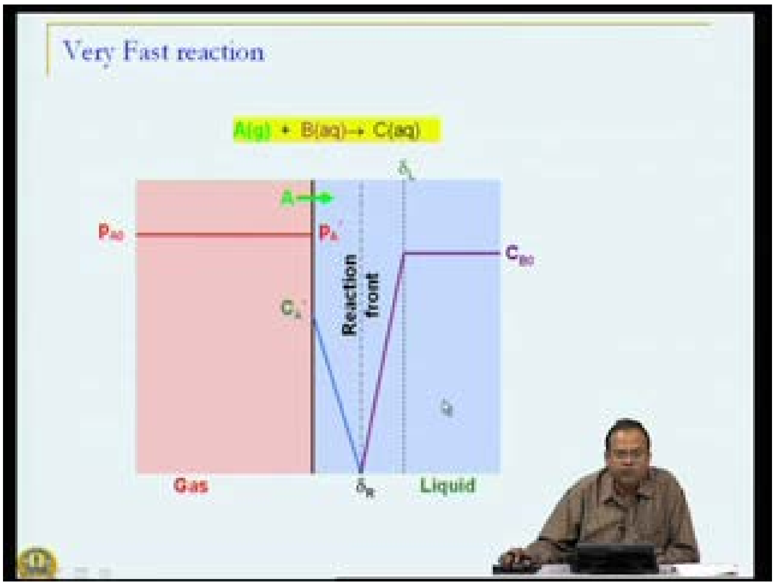

Very Fast reaction

$A(g) + B(aq) \rightarrow C(aq)$

So if you make this reaction even more fast that is very fast. Let us say then there will be a point for example, if we look at this particular case if the reaction is slightly faster then what will happen is that a will get depleted even earlier and earlier and there will be actually two fronts. Two fronts where on one side A is getting depleted on other side B is getting depleted and reaction is so fast that as soon as A and B comes into contact with each other. This species will react and leading to concentrations of A and B close to zero at some location delta R or in other words the reaction now would not be occurring in these entire boundary layer but almost along this reaction front or along the plane that is not in the volume of these boundary.

But along the plane which defines this boundary. Now initially this front will be located at y equal to delta L and as reactions go on becoming faster and faster this front will move towards the gas liquid interface and the reaction will stop when the concentrations go to zero at this particular inter phase itself.

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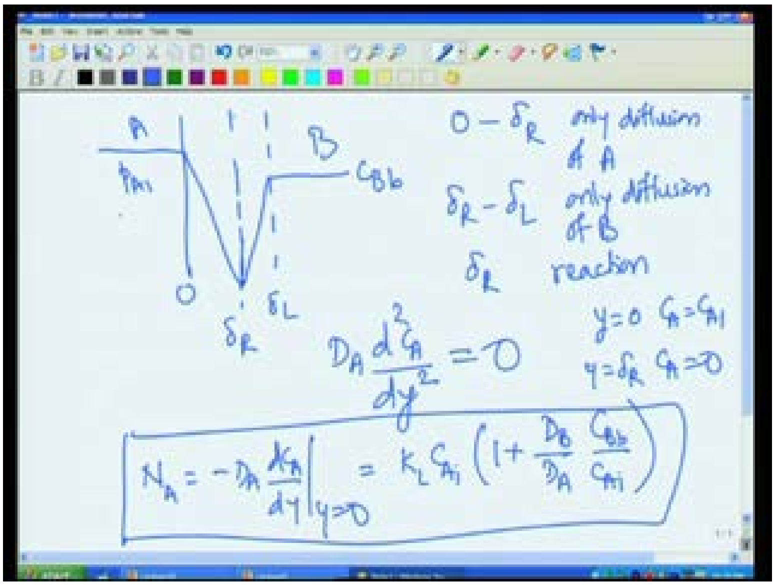

$0 - \delta_R$ only diffusion of A

$\delta_R - \delta_L$ only diffusion of B

δ_R reaction

$y = 0$ $C_A = C_{Ai}$

$y = \delta_R$ $C_A = 0$

$$D_A \frac{d^2 C_A}{dy^2} = 0$$

$$\boxed{N_A = -D_A \frac{dC_A}{dy}\bigg|_{y=0} = k_L C_{Ai}\left(1 + \frac{D_B}{D_A}\frac{C_{Bb}}{C_{Ai}}\right)}$$

So, let us just quickly look at how do we analyze this situation and write down the relevant mass balances to see how we define this system. So let us say that we have our hydrodynamic… We have our inter phase hydrodynamic boundary layer delta L and what is happening to the gas is that the gaseous component is getting dissolved and at this location both A and B goes to zero. That is this is the front at which the reaction is occurring so reaction front. So this is my A, this is my B, this is some bulk concentration of B and this is some partial pressure at the inter phase. So what we have now here is between zero to delta R only diffusion of A because there cannot be any reaction because at this point there is no B left.

So there is only diffusion of A whereas between delta R and delta L there is only diffusion of B and at delta R there is a instantaneous reaction. So diffusion on these two between zero to delta R and delta R to L and reaction at delta R. So in this particular case we can set up the mass balances just as we did earlier that is namely for A for example, if you look this is the diffusion and there is no reaction between zero to delta R and the limits are at y equal to zero C A is equal to C A I, which is in equilibrium with the gas and at y equal to delta R C A is equal to zero.

A similar mass balance can be written for B and if we do all this if we do all these things, then we can then find out our flux which was minus D A dC A dy at y equal to zero and this comes out to be… That is if you solve mass balances for A and B and use appropriate boundary conditions we will end up with the flux that is as we are standing in the gas phase, what is the rate of absorption of observed rate of absorption of A in the liquid?

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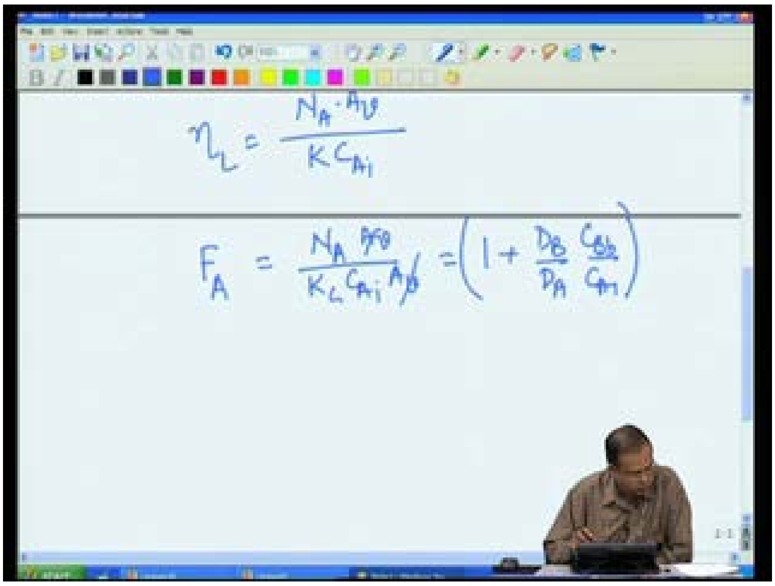

$$\eta_L = \frac{N_A \cdot A_V}{K C_{Ai}}$$

$$F_A = \frac{N_A \cancel{A_V}}{K_L C_{Ai} \cancel{A_V}} = \left(1 + \frac{D_B}{D_A}\frac{C_{Bo}}{C_{Ai}}\right)$$

So this is given by this particular expression and we can then immediately see we can go on then to define for example, effectiveness factor that is effectiveness factor which is, what is my flux actual observed flux to what would have been the flux if there was no mass transfer limitation? Same thing as before as well as we can define our enhancement factor F A or E as what is my observed flux to what would have been the flux if there was only mass transfer. So we can put area in both cases but those will get canceled out. So, what would have been the flux and from this flux equation that is nothing but that would have been my effectiveness or enhancement factor. So depending upon the values of the bulk concentrations and their diffusivities I will have different values of effectiveness factor.

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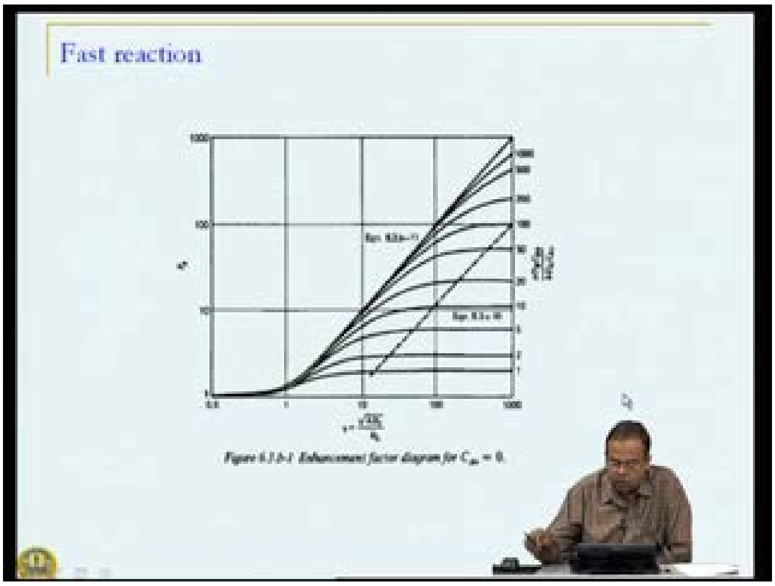

Fast reaction

Figure 6.3.b-1 Enhancement factor diagram for $C_{Bs} = 0$.

So essentially the idea is that if you have a very fast reaction, the reaction is restricted only to the plane and then we can get various enhancement factors and this is what is actually shown in this particular figure. The top figure was for moderate reaction and these are the different values that you will get depending on the value of this dB by dA and so on. So these are this is how enhancement factor diagrams will look like for a fast reaction.

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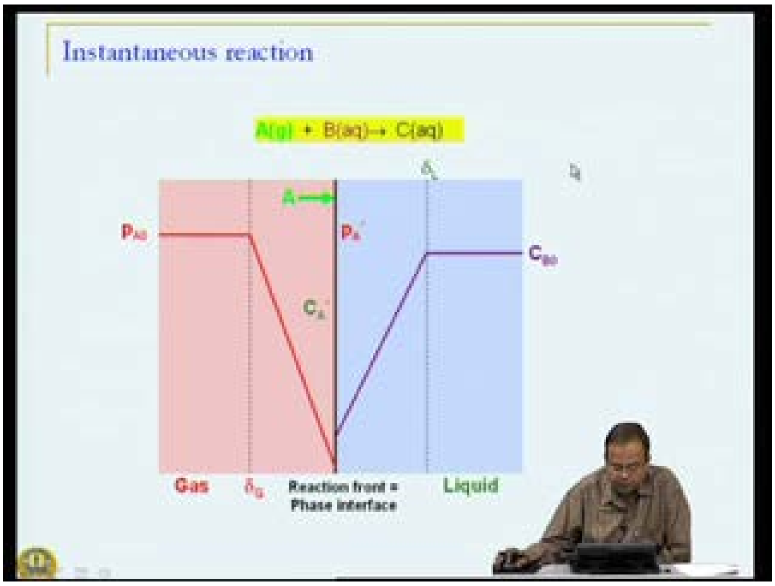

Instantaneous reaction

$A(g) + B(aq) \rightarrow C(aq)$

With this, we now come to the conclusion of our discussion on gas-liquid reaction, and in general on discussion on heterogeneous reactions. To recap what we started out with after we had a brief review of undergraduate chemical reaction engineering. We looked at different complex kinetics. So, our first module if you like to call it was focused on looking at the complex kinetics, and what are the different scenarios where one gets these complex kinetics. So we had catalysis, we had chain reactions, and different types. But more than that we focused on how do we analyze complex reactions.

How do we get the kinetics when the reactions number is large or species are unknown and so on. So that was mainly our module one. In the second module, we looked at the heterogeneous reactions that is reactions when there are more than one phase present and as a result of phases there are boundaries and because there are boundaries there is a mass transfer or energy transfer limitations and we saw how these influence the kinetics of the process that is what essentially the transport phenomena what role does it play in determining the kinetics.

Now all that we now need to know to complete our discussion on chemical reaction engineering is to now actually put this two together, that is the kinetics and heterogeneous reactions into our reactor and look at how reactor behavior is influenced by either the kinetics or by the transport phenomena or by the characteristic of the reactor itself. We had briefly talked about design equations for reactors but those were mainly for ideal reactor, plug flow reactor or continuously stirred tank or continuously stirred reactor where there is very good mixing or anything in between.

What at that point of time we did not pay much attention to for example, heat effects of chemical reactions. So we never for example, discussed about non-isothermal reactor. So those are some of the things that we will now discuss in our third module, which will be the concluding module for this particular course. It will run I think for another ten to fifteen lectures where we will do mix of things. I will start out by formulating general mass and energy balances for the reactor and then look at the behavior of non-isothermal reactions. Because they lead to quiet a interesting set of behavior and look at design of few reactors taken from industrial practice.

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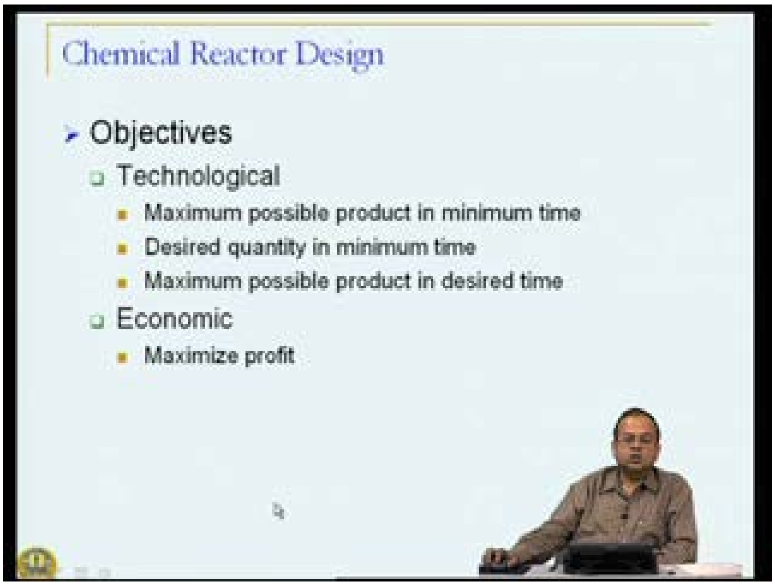

Chemical Reactor Design

- Objectives
  - Technological
    - Maximum possible product in minimum time
    - Desired quantity in minimum time
    - Maximum possible product in desired time
  - Economic
    - Maximize profit

So, let us begin our discussion on looking at the reactor design. So what are the basic ideas in reactor design, just general background before we go into the detail discussion on reactor design. Now when we say we want to design a reactor we must be absolutely clear as to why are we designing this reactor? What are our objectives? So any reactor design or for that matter any design activity always has to start with well defined objectives. So, what are the possible objectives in a chemical reactor design? It turns out that there are several types of objectives that may come into picture.

For example, our objectives may be technological in nature that is purely technology kinetics and so on. So it says that maximum possible product in minimum time that is one kind of a technological objective. It may not be always maximum possible but you have certain desired quantity in mind. So achieve that in minimum time. So you may be able to make more than that but maybe the time required is more. So you be happy with the desired quantity in absolutely minimum time. Maximum possible product in desired time is other way of looking at the same problem. So these are all technological in nature these objectives but the real objective in any commercial operation are the economic objectives that is maximized profit as simple as that.

Now that may take the form of maximizing either productivity or maximizing yield that is technological aspect. But bottom line anybody who wants to design and run and make some commercial venture out of a chemical reaction the objective is maximized profit. While we talk about these objectives I want to also emphasize that it is not that the design is always done with a single objective in mind because even if you want to maximize profit you also now are required to minimize losses. That is there should not be any effluents coming out of your plant dumping anything in the aqueous environment or in the air and so on.

So your objective actually could be maximizing profit while minimizing the environmental impact. So it is a multi objective problem. So more often than not one comes across situations where there are two objectives that one wants to meet and it is many times it is not possible that both these objectives will be meet in the in simultaneously. So there has to be a tradeoff and therefore, we have various multi optimization or multi objective optimization strategies designed to look at these kinds of problems. Defining objective is only the starting point, the second point that or second aspect that we have to focus on how do I achieve these objectives.

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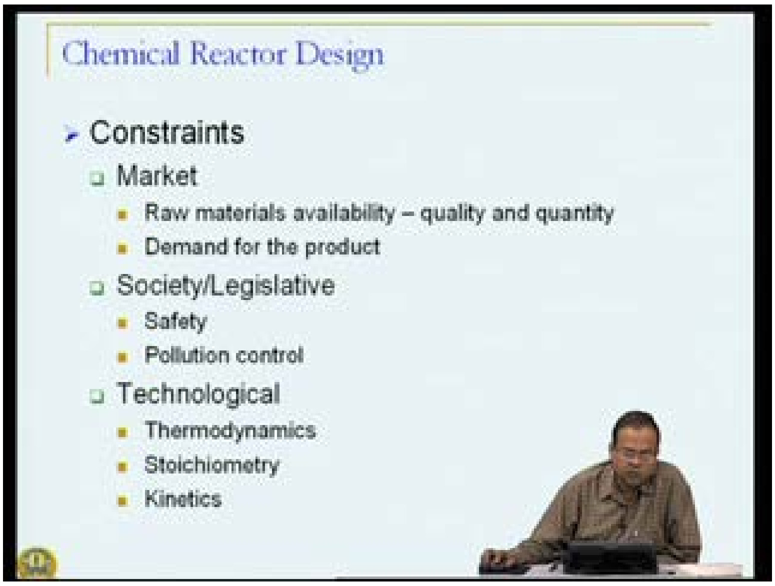

Chemical Reactor Design

- Constraints
  - Market
    - Raw materials availability – quality and quantity
    - Demand for the product
  - Society/Legislative
    - Safety
    - Pollution control
  - Technological
    - Thermodynamics
    - Stoichiometry
    - Kinetics

That means what are the things that I decide, so that I can achieve these objectives or in other words what are my decision variables? Before we go to decision variable I want to go back to my objectives and these objectives would not be difficult to achieve if there were no constraints on our system. So what are those constraints so while defining the reactor design objective, we must be aware of what are the constraints under which we are working. So there are various different types of constraints and I will start with market forces first raw material availability.

For example, if you want to design something starting with natural gas your likely preference would be the source of natural gas, wherever it is available because you do not want to transport gases gas over a long distance although that is being done. But your preference still would be that you either you have it on the coastal region or wherever there is a ready available source and that is applicable to all other industries also that is availability quality quantity and so on is a constraint. So within that you have to work. Then the demand for product, you may have a wonderful product but if there is no demand there is no design.

Then there are more important societal or legislative constraints safety for example, is the prime constraint that has to be satisfied. You cannot compromise on that otherwise you will pretty soon go out of business. Pollution control, so zero discharge policies as implemented by several societies so that is your constraint so you may have a wonderful product, you are may be able to get wonderful yields from it but while doing so, if you are generating undesirable waste that process is not going to take you anywhere. So while designing itself developing the process itself one must be aware of what is the constraint under which I am working.

Am I allowed to discharge this much material in the aqueous stream or what are the costs in world if I have to treat this material? So all that has to now come into your design criteria and lastly but not the least important that is actually what will give you the product desired product or the technological constraints. We studied about thermodynamic stoichiometry kinetics in the first module of this session. But another way of looking at these thermodynamic considerations is look at them as constraints. See I may desire that I want ninety percent conversion of my reactant. But thermodynamic dictates that the equilibrium conversion is only sixty percent.

So how do I go from 60 percent to ninety percent? First of all left to it you cannot do anything about it. So thermodynamics has become your constraint is there any way of overcoming this constraint? Yes. You may have a separation scheme where you continuously keep removing product. So that your thermodynamics is now equilibrium shifted towards making of more products. So but whatever is the solution there is a constraint, stoichiometry is another constraint. I may want thousand kilograms of certain product but then stoichiometry dictates that unless I spend some two thousand kilograms of something else, I may not be able to generate the thousand kilograms of desired material or all those stoichiometry coefficients.

One mole of this combines with two moles of that to give you one mole of this that kind of reactions that we saw. So to make one mole of product you may have to require two moles of reactants or one mole of certain reactant two moles of certain other reactant and so on. And lastly the kinetics, now in deriving any a maximum profit out of your process or increasing the productivity you would be rather impatient. You would like that reaction to be as fast as possible instantaneous if it is left to you. So moment you have two reactants coming in contact they react give you wonderful product.

Unfortunately, kinetics of the process has it is own limitations. Even without any mass transfer or heat transfer limitations the reactions have some finite rate as we saw, which depends on temperature concentration and so on. So that is, what is the constraint on your process now? Then you have mass transfer putting additional constraint. For example, if it is a heterogeneous reaction your mass transfer itself may become limiting or putting limitation on how fast you can drive the reaction and so on. So all these factors now became constraints for us. So, we have objectives we have these constraints under which we are working. So, how do we meet our desired objective while restricting ourselves within these constraint domains? How do we do that?

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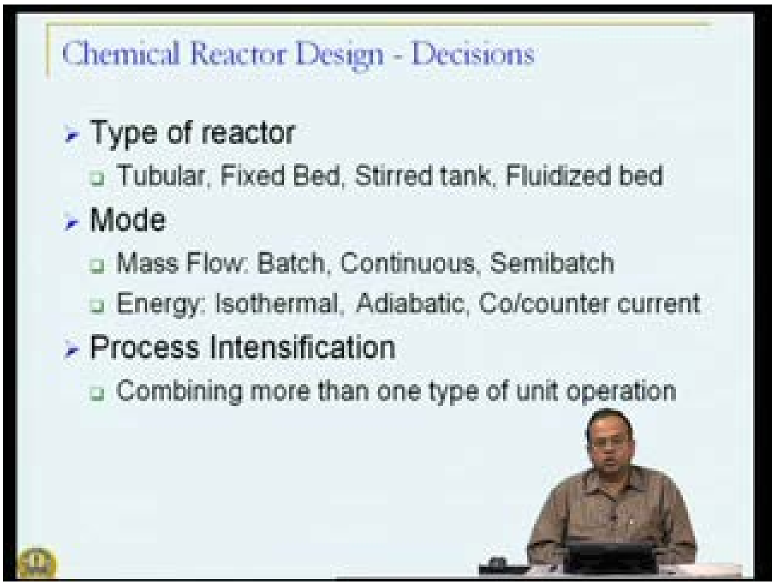

Chemical Reactor Design - Decisions

- Type of reactor
  - Tubular, Fixed Bed, Stirred tank, Fluidized bed
- Mode
  - Mass Flow: Batch, Continuous, Semibatch
  - Energy: Isothermal, Adiabatic, Co/counter current
- Process Intensification
  - Combining more than one type of unit operation

So, what are the decisions that we take. There are certain types of decisions that we often make and one of the foremost for example, is what kind of reactor we choose. We choose a tubular reactor or a fixed bed reactor, stirred tank reactor, fluidized bed reactor for a given process. Now that will depend on what kind of process is it for example, tubular or I mean if it is a gas-solid process, fixed bed reactors or fluidized bed reactors are likely candidates. Now how whether we go for tubular or stirred tank or fixed or fluidized there equivalent counter parts for that solid reactions will be determined by what is the kinetics of the process.

If you recall in our initial discussion, we saw that often for first order reaction for example, tubular reactor will give you a higher conversion. But we also saw a case where if it is not the conversion but the selectivity is what is of importance, then stirred tank reactor may give you better selectivity than plug flow so all these decisions will have to be made. Second set of decisions that we have to make is how we operate this reactor.

What is the mode of operation? Do we operate it as mass flow that is in terms of batch continuous or semi batch process or in terms of energy flow?

That is isothermal, adiabatic, co current or counter current or what kind of operation do we do and of course, of let there is another kind of decision that that has become equally important process intensification how do I get most out of my existing. So can I combine more than one process one that is reaction and separation into a single step or any other means of process intensification.

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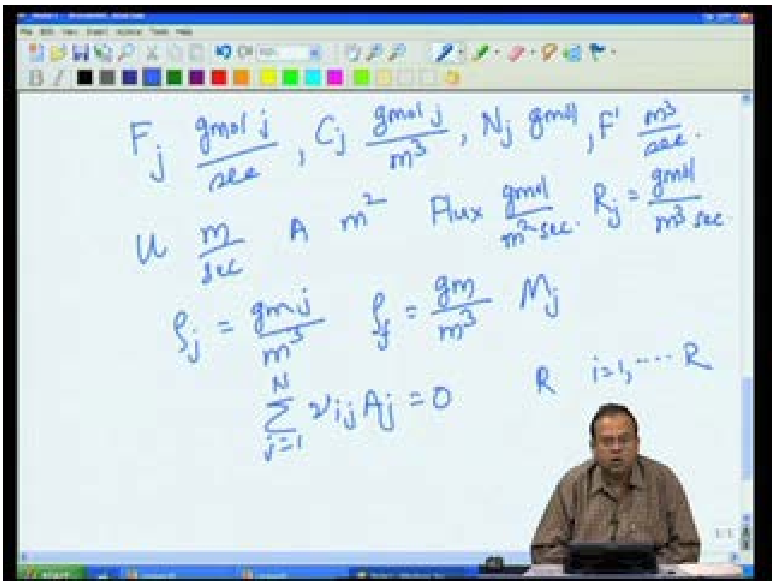

$F_j \ \frac{gmol\ j}{sec}$, $C_j \ \frac{gmol\ j}{m^3}$, N_j gmol, $F' \ \frac{m^3}{sec}$.

$u \ \frac{m}{sec}$ $A \ m^2$ Flux $\frac{gmol}{m^2\,sec}$. $R_j = \frac{gmol}{m^3\,sec}$

$\rho_j = \frac{gm\ j}{m^3}$ $\rho_f = \frac{gm}{m^3}$ M_j

$$\sum_{j=1}^{N} \nu_{ij} A_j = 0 \qquad R \quad i = 1, \cdots R$$

So, now let us given this background let us start discussing about the reactor design and we will do this start this by considering simple mass balances and energy balances for stirred tank reactors, tubular reactors and so on. So we will just take a brief overview of these design equations and then move on to the actual examples of few reactor behaviors. So, before we get into the material itself just a word about different terminology that we will be using. For example, F j as gram mole of j per second that is molar flow rate I am just repeating some of these scenes, we had seen earlier but for sake of clarity let us let just repeat this once again.

So F j is the molar flow rate; C j is the concentration gram mole of j per meter cube let us say the units whether they are in decimeter cube or meter cube or centimeter cube is left to you but essentially this is what we do. N j number of moles so just gram mole, so molar flow rate concentration and molar flow rate flow rate concentration moles and one more volumetric flow rate, so F prime as meter cube per second let us say so it is not very difficult to see that C j into F prime is F j that is how we define few more set of notations, u the velocity meter per second let us say.

A meter square cross sectional area then we will use flux, which is gram mole per meter square second R j rate of reaction, so gram mole per meter cube per second. Then rho j the density gram of j per meter cube let us say, rho f the density of the entire reacting mixture rho j is the density of the jth species. So this we can define as gram per meter cube and then molecular weight M j and so on. What we are interested in looking at set of reactions in species A j. So j goes from one to j goes from one to N and there are R such independent reactions i equal to one two up to R. So this is what we are going to look at and to begin with we will start with homogeneous reaction in a tubular reactor.

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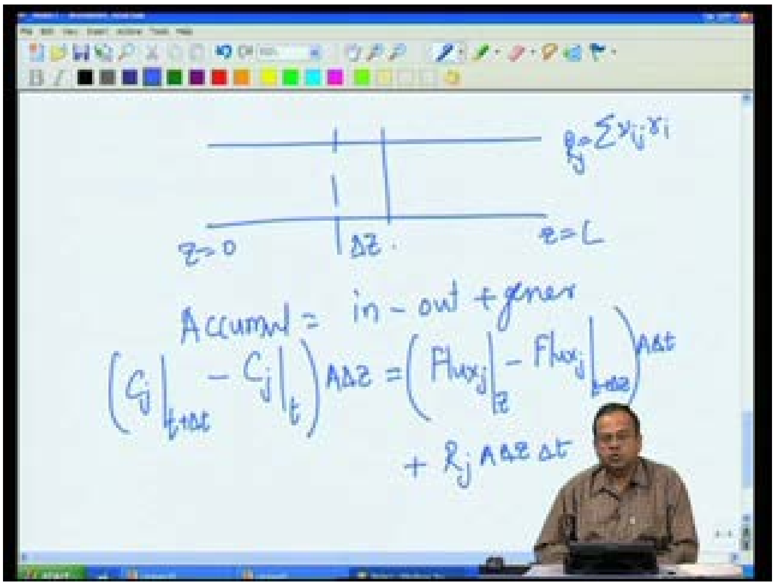

$R_j = \sum \nu_{ij} r_i$

Accumul = in − out + gener

$$\left(C_j\Big|_{t+\Delta t} - C_j\Big|_t\right) A\Delta z = \left(Flux_j\Big|_z - Flux_j\Big|_{z+\Delta z}\right) A\Delta t$$
$$+ R_j A\Delta z\, \Delta t$$

So, essentially although we will not repeat this exercise again and again the idea is you have a tubular reactor; you look at the cross-sectional delta z. So let us say this is its entry point, this is the exit point and you are looking at cross section delta z. Then we write a simple mass balance accumulation equal to whatever is coming in minus going out plus generation. So we can then use all the appropriate terminologies to represent accumulation and I am going to write this only once. So that we do the similar exercise at for everything else so if C j is the concentrations the mass balance is in terms of mass, so moles not in terms of concentrations.

So whatever was present at time t plus delta t minus whatever was present at time t means the mass, which is accumulated and since I am doing it in terms of mass it has to be multiplied by the volume, which is A delta z will be whatever is coming in. So let us write down this in terms of flux of j at z minus going out flux of j at z plus delta z and this flux so to get moles multiply by area and flux as time, so this happening in small time interval delta t is what represents my in and out term and the rate of reaction R j for the for the species j, R j is not rate of any one particular reaction but R j is the rate of change or generations of j th species.

If you recall that was nu i j r i this is my R j that is r i is the rate of i th reaction stoichiometric coefficient for jth species this is nu i j. So summed over summed over all such reactions for j th species give me R j but this is per unit volume and per unit time, so A delta z delta t. So this is my simple mass balance which we now divide by delta z delta t take a limit as delta z goes to zero, delta t goes to zero.

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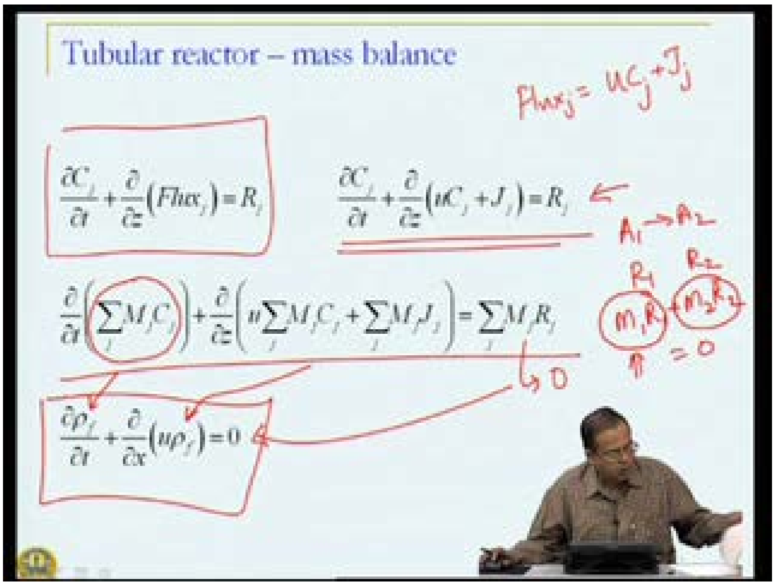

Tubular reactor – mass balance

$Flux_j = uC_j + J_j$

$$\boxed{\frac{\partial C_j}{\partial t} + \frac{\partial}{\partial z}(Flux_j) = R_j}$$

$$\frac{\partial C_j}{\partial t} + \frac{\partial}{\partial z}(uC_j + J_j) = R_j$$

$A_1 \rightarrow A_2$

$R_1 \quad R_2$

$m_1R_1 + m_2R_2 = 0$

$$\frac{\partial}{\partial t}\left(\sum_j M_jC_j\right) + \frac{\partial}{\partial z}\left(u\sum_j M_jC_j + \sum_j M_jJ_j\right) = \sum_j M_jR_j$$

$\rightarrow 0$

$$\boxed{\frac{\partial \rho_j}{\partial t} + \frac{\partial}{\partial x}(u\rho_j) = 0}$$

We will end up with this kind of mass balances and here we are going to look at only final set of equations. So that discussion proceeds at a reasonable rate detailed derivations you can find in any standard textbook. So for example, the first set of equation that we get is our mass balance equation from the same balance that we wrote dou dou t of C j and partial equation because both time and axial coordinate is considered or special coordinate is considered. So both equation in time and space domain so we have partial differential equation unsteady state balance into flux of j equal to R j and what is this flux of j?

There are two forces that are responsible for flux one the convective flux which is u into C j plus diffusive flux which is J of j so this flux in my mass balance can be represented in this particular manner. So now if I do the summation that is multiply these equation by M j and summed it over all species, you get this kind of equation which you can see summation M j C j, M j is the molecular weight C j is the moles of moles of species j. So this is nothing but density of my fluid rho f, this is nothing but u rho f and summation M j R j.

See when you have a stoichiometric reaction let us say A 1 going to A 2 then rate of reaction for R 1 A 1 is let us say R 1 for A 2 is R 2 if you multiply M 1 by R 1 plus M 2 by R 2, this must add up to zero, why because this is what is the mass of A 1 that is disappearing. This is, what is the mass of A 2 that is appearing in this particular reaction? So that net sum of these two must be zero. Because you are not going to generate mass out of nowhere the reason why A 2 is getting formed is because A 1 is getting consumed. So we have loss of A 1 which results into generation of A 2, so not in terms of moles.

But in terms of mass that is why we will multiply by molecular weight their addition must be zero and this is applicable even more general you have any n number of species which are getting generated at a rate R 1 then summation over all those species must be equal to zero. So if that is the case we end up with these equations and this equation is nothing but the continuity equation even for a non reacting species. So even for reacting species the continuity equation remains the same that you must have seen in your transport course when you deal with such course.

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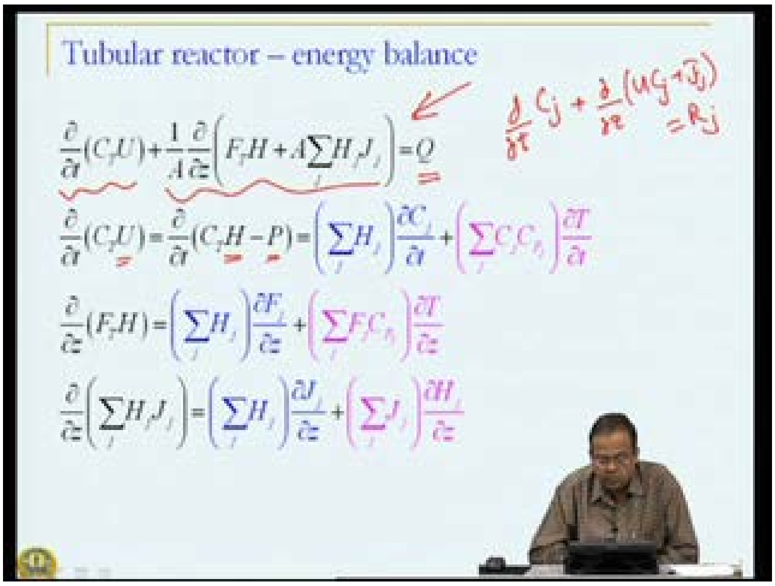

Tubular reactor – energy balance

$$\underline{\frac{\partial}{\partial t}(C_T U)}+\underline{\frac{1}{A}\frac{\partial}{\partial z}\left(F_T H + A\sum_j H_j J_j\right)}=\underline{\underline{Q}}$$

$$\frac{\partial}{\partial t}C_j+\frac{\partial}{\partial z}(uC_j+J_j)=R_j$$

$$\frac{\partial}{\partial t}(C_T \underline{U})=\frac{\partial}{\partial t}(C_T \underline{H}-\underline{P})=\left(\sum_j H_j\right)\frac{\partial C_j}{\partial t}+\left(\sum_j C_j C_{pj}\right)\frac{\partial T}{\partial t}$$

$$\frac{\partial}{\partial z}(F_T H)=\left(\sum_j H_j\right)\frac{\partial F_j}{\partial z}+\left(\sum_j F_j C_{pj}\right)\frac{\partial T}{\partial z}$$

$$\frac{\partial}{\partial z}\left(\sum_j H_j J_j\right)=\left(\sum_j H_j\right)\frac{\partial J_j}{\partial z}+\left(\sum_j J_j\right)\frac{\partial H_j}{\partial z}$$

Now let us try to look at energy balance, and energy balance is slightly more involved. But I think there is a analogy that one can always draw, let me see if it I have indicated it here. If you recall our mass balance which we saw just few minutes back a corresponding energy balance for the reactor would be can be written, and this is actually equation taken from vanish and smith for internal energy balance. It is the same thing accumulation of energy the flux, and the rate of addition or removal of heat Q. Now it turns out that we actually do not see any reaction term over there, and for which you have to actually write internal energy u as enthalpy C T H minus P, that is C T U is C T H minus P.

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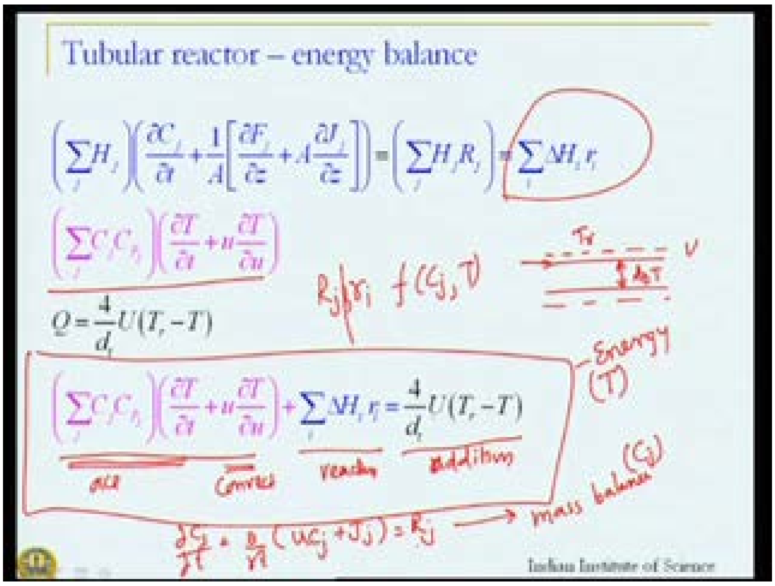

Tubular reactor – energy balance

$$\left(\sum_j H_j\right)\left(\frac{\partial C_j}{\partial t}+\frac{1}{A}\left[\frac{\partial F_j}{\partial z}+A\frac{\partial J_j}{\partial z}\right]\right)=\left(\sum_j H_j R_j\right)+\sum_i \Delta H_i r_i$$

$$\underline{\left(\sum_j C_j C_{pj}\right)\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial z}\right)}$$

$$Q=\frac{4}{d_t}U(T_r-T)$$

$$\boxed{\underbrace{\left(\sum_j C_j C_{pj}\right)\left(\frac{\partial T}{\partial t}\right.}_{acc}\underbrace{\left.+u\frac{\partial T}{\partial z}\right)}_{convec}+\underbrace{\sum_i \Delta H_i r_i}_{reaction}=\underbrace{\frac{4}{d_t}U(T_r-T)}_{addition}}$$

$$\frac{\partial C_j}{\partial t}+\frac{\partial}{\partial z}(uC_j+J_j)=R_j \longrightarrow \text{mass balance } (C_j)$$

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And if you go on simplifying or expanding these terms we actually get this kind of equation. That is all we are doing is expanding these terms and finally, we are left with the following equation summation H j into delta C j delta t plus 1 over this particular term. This actually if you notice is nothing but our reaction term. So if you take this particular term this simplifies to this summation delta H i r i. Then the first term simplifies to this. So we have this plus delta H i r i and if you say that suppose we have our tubular reactor and it is a saline tube kind of arrangement the diameter is let us say dt the heat transfer coefficient.

let us say is U and there is a fluid at a temperature T r flowing through this cell side reaction is occurring in the tube side, then the heat added to the system is one can show is four by dt U into T r minus T. So, if T r that is a temperature outside is greater than the temperature in the reactor the heat will be added and if it is other way round there will be cooling. So what do we have here we have the energy accumulation term, the convective transport term, the reaction term. What is the rate of generation of energy and addition energy addition term? So this is the comprehensive form of energy balance equation for a tubular reactor.

So when we deal with mass and energy balance we have to consider this energy balance along with our mass balance equation. Now I will write down the mass balance equation once again just to highlight the fact that highlight the following fact. So this is my energy balance, this is my mass balance. So this is the balance it is not a balance on temperature, it is a balance on energy but the variable that appears in that balance is temperature because we define energy as C P delta T or change in energy or C P delta T and so on. So we have this temperature and mass balance as this concentration.

Again it is a mass balance not a concentration balance but after certain simplifications we get this kind of behavior. Now if you look at these two equations these are highly coupled equations why because first of all R j or for that matter r i which appear in these two places these are functions of C j and T, both are functions of functions of C j and T. So how C j changes depends on temperature and how temperature changes depends on the concentrations. So these are not uncoupled equations so mass and energy effects have to be considered together and not in isolation of each other.

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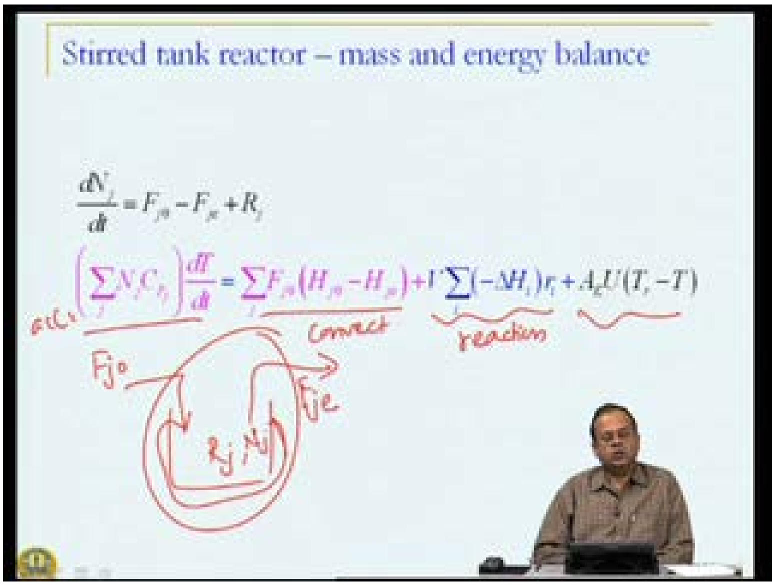

Stirred tank reactor – mass and energy balance

$$\frac{dN_j}{dt} = F_{j0} - F_{je} + R_j$$

$$\left(\sum_j N_j C_{pj}\right)\frac{dT}{dt} = \sum_j F_{j0}(H_{j0} - H_{je}) + V\sum_i(-\Delta H_i)r_i + A_k U(T_c - T)$$

For a stirred tank reactor, these balances simplify to this particular set of equation. That is what we have now is we have the molar flow rate entry exit of the j th species. R j is the reaction rate and N j is the number of moles here. So d A i N j dt is equal to coming in going out plus R j. So we now have a balance over the entire reactor. Because it is a stirred tank reactor there are no variations and similar energy balance this is the energy content of the reacting mixture. So this is the energy accumulation, this is convective flow in and out so enthalpy of the stream coming in minus enthalpy of the stream coming out. This again is the contribution due to reaction.

So this is convection, this is accumulation the energy and this is if you have a reactor with a jacket, what would be the rate of it addition. So in this particular case A k is the area of jacketed area, U is the transfer coefficient T r minus T, T r is the reference temperature T is the temperature inside. So once again if we are passing hot fluid in the jacket we will have heating; if we are passing cold fluid we will have cooling. So this is how stirred tank reactor mass and energy balance equations look like. These are just reactors where we assumed that that there is no heterogeneous phase or only single phase.

Now one may ask question what happens if you have heterogeneous reaction that is when you have two phases multi phase situation. So this is something that we will see in our next session that how we represents a heterogeneous phase while taking into account or while looking at design of a heterogeneous reactions. So before I conclude this session what we actually did today was to conclude our discussion on gas-liquid reactions and thereby general discussion on heterogeneous reactions.

So, we looked at today in particular case where the reaction is so rapid or instantaneous that it is confined to a plane rather than the volume either in the bulk or in the boundary layer. And then we started discussing about reactor design by focusing on what are the important considerations in reactor design, and looking at the mass balance equations for tubular reactor as well as for a stirred tank reactor. So in the next session, we will look at what happens when we have heterogeneous reactions that is either gas-solid catalytic or non-catalytic reactions, and how do we account for the presence of these two phases in developing the mass, and energy balances. So, that will be the topic for the next session. Thank you.