# Chemical Reaction Engineering

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## Lecture No. # 28

## Chemical Reactor Design: Mass and Energy Balances for Heterogeneous Reactions

Friends, let us continue our discussion on reactor design and before we go to some few specific cases of different types of reactors. Let us just recap what we saw in the last session namely the mass and energy balances for tubular and stirred tank reactors when we are dealing with homogenous system.

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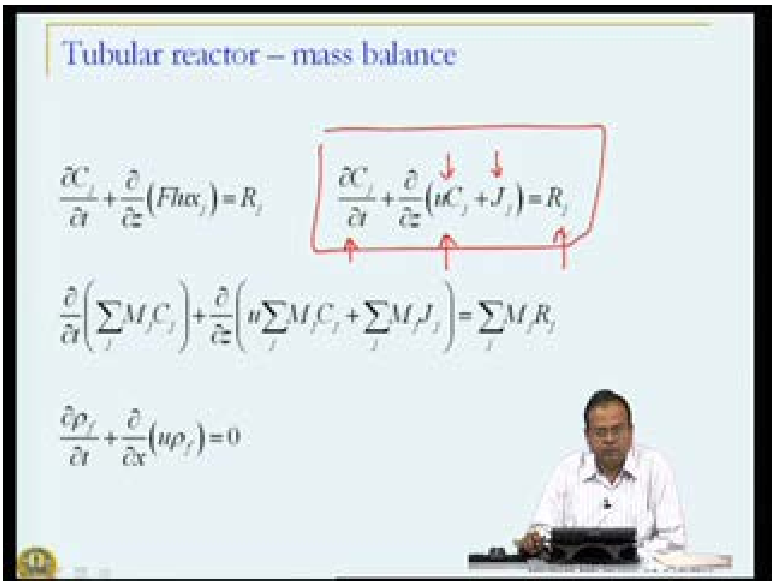

Tubular reactor – mass balance

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

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

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

So starting with tubular reactor and mass balance equations, we have this mass balance equation and if we are please note we are dealing with homogeneous system. So this is our mass balance equation which denotes for accumulation term denotes for the fluxes, which are both convective as well as diffusive at the rate of generation of the species. So this is our mass balance equation for a tubular reactor.

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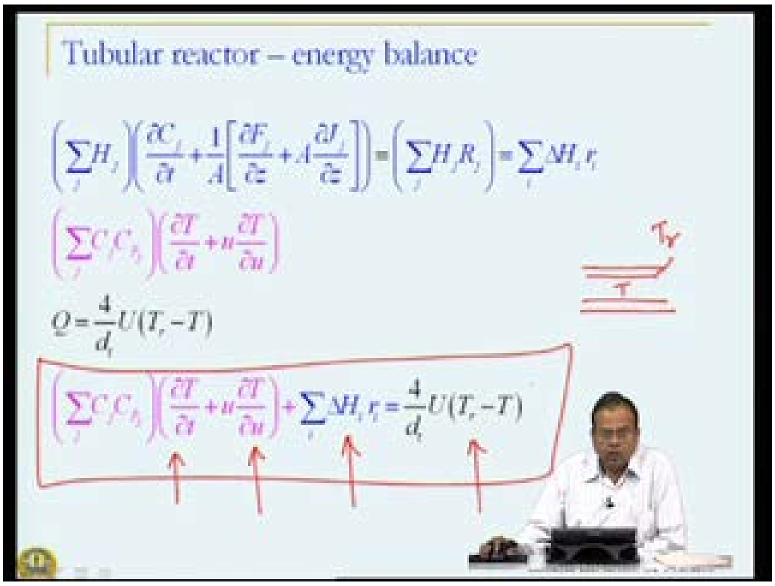

Tubular reactor – energy balance

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

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

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

$$\boxed{\left(\sum_j C_j C_{p_j}\right)\left(\frac{\partial T}{\partial t}+u\frac{\partial T}{\partial u}\right)+\sum_i \Delta H_i r_i=\frac{4}{d_t}U(T_r-T)}$$

Now if we go through energy balance we once again have a similar energy balance. The first term here denoting the accumulation of energy, this is the convective flux or convective enthalpy flow if you like to call it. This is the contribution due to reaction summation delta H i r i that is if we assume that there are N reactions i 1 2 3 4 up to R reactions let us say independent. Then each of this reaction is having heat of reaction delta H i then sum total of delta H i and r i will be the net generation of energy in the reactor and the last term accounting for the energy that is added to the system.

For example, this is this is assuming that we have a tubular reactor and it is surrounded by a shell through which a cold or hot fluid at reference temperature T r is flowing through. So depending upon weather T r is greater than T that is temperature inside the reactor either will have adding the energy to the system or we will be removing the energy to the system.

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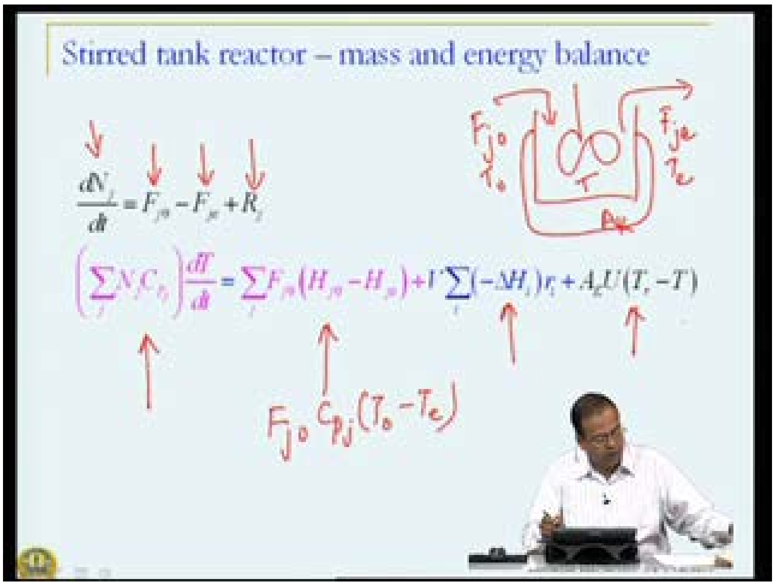

Stirred tank reactor – mass and energy balance

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

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

$$F_{j0} C_{p_j} (T_0 - T_e)$$

Now this is as for as the tubular reactor is concerned for stirred tank reactor. We can write mass and energy balances that is what we have here is a stirred tank reactor with material flowing continuously in and out. Let us say for the j species these are the flow rates temperature inside is T let us say that let us say that temperature here is T naught here is T e same as T. So once again accumulation is molar flow rate coming in going out plus what is getting generated that is our mass balance for stirred tank reactor. Similar energy balance energy accumulation this is the convective enthalpy flow, which as you would guess at some point assuming constant c p can also be written as T zero minus T e more familiar term.

This is the contribution due to reaction and this is the heat addition to the system. Once again we have a jacket having a cross area of coverage A k transfer coefficient u so T r minus T that becomes our energy balance. Now let us move forward and see what happens to our mass and energy balances when we have multiphase systems and in particular we would like to look at what happens to mass and energy balances when we have gas solid catalytic reactions let us say non-catalytic reactions will be also along the similar like.

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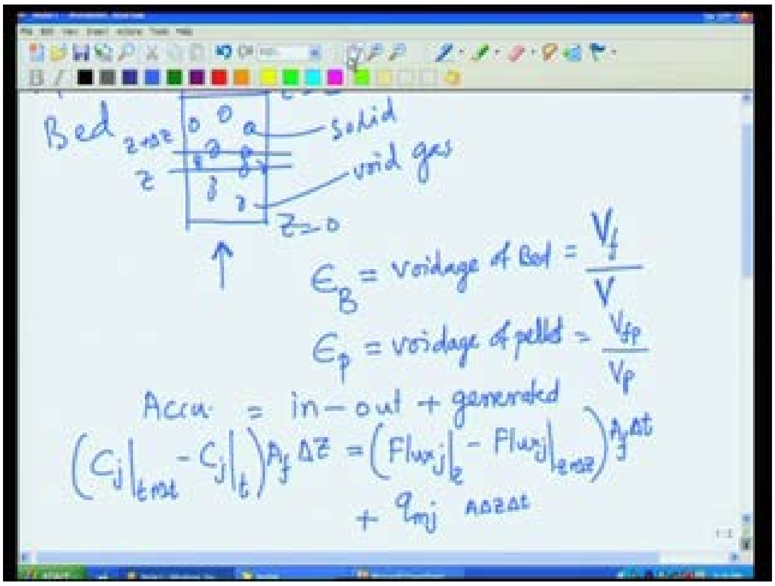

$\epsilon_B$ = voidage of Bed = $\frac{V_f}{V}$

$\epsilon_p$ = voidage of pellet = $\frac{V_{fp}}{V_p}$

Accu = in − out + generated

$$\left(C_j\big|_{t+\Delta t} - C_j\big|_t\right)A_f\,\Delta z = \left(\text{Flux}_j\big|_z - \text{Flux}_j\big|_{z+\Delta z}\right)A_f\,\Delta t + q_{mj}\,A\,\Delta z\,\Delta t$$

So let us try to first look at how we developed the mass balances for gas-solid catalytic reaction. So we are now considering multiphase reactors and let us start with fixed bed reactor and extensions for other kinds will follow in due course. So let us say that this is my reactor it is part with solids between z equal to zero to z equal to l. So there are solids all through this all through this reactor. The gaseous components come inside the reactor they react in presence of this catalyst and they leave. Now this also in some sense is a tubular reactor although in tubular reactor we always show it like this no nothing prevents us from showing tubular reactor in this particular manner, the orientation hardly manners matters.

It is the kind of flow that that flows inside these reactors which is of concern to us. So in principle the mass and energy balances for fixed bed reactor. So we are looking at fixed bed reactors now must be same as or similar to at least that of tubular reactor indeed they are however there is one difference that we have to we have to take into account and that is there are two phases in this reactor one solid and other one the void or the gaseous phase, which represents the voids. Now our gaseous reactants are moving through the voids then they are getting diffused or they are diffusing inside the catalyst reacting products are coming and so on.

But as far as the main flow is concerned convective flow is concerned. It is essentially from one end of the reactor through voids of this bed through to the other end of the other end of the reactor. So in this particular case we have to now consider or acknowledge the presence of these solids in this in this reactor. So to do that let us start defining few quantities. Let us say that epsilon B is the void age of the bed that means the volume that is available for gases to flow V f to the reactor volume V, let that be epsilon p. Then we also have to worry about the void age in the catalyst pore because remember the catalyst is also porous.

So let us call epsilon p as the void age of the catalyst pellet which is V f p void volume of the pellet divided by the volume of the volume of the pellet. So now let us let us try to write down the mass and energy balances for this particular reactor starting with let us say that we have a small cross section of z and z plus delta z of this bed and let us try to look at what is happening in this small cross section. So what is this small cross section it consist of both solids and the voids and we will assume that void fraction is uniform through the bed.

So epsilon B equal are applicable in this particular case as well. So let us try to write down the mass balance equation for the component j which is part of this reacting string so as before we will do accumulation equal to in minus out plus generated so same as same as before. Now let us look at accumulation term. If we say that C j concentration at time t plus delta t and C j at time t is the concentration at time t. Then this into A f into delta z that is the volume. Remember the concentration C j is per unit per unit fluid volume multiplied by the fluid volume is the total moles of j which are which are accumulated.

Now this accumulation is result of flux of j that is coming in at z minus flux of j at z plus delta z in time delta t and flux is again in void volume per unit void area sorry. So that is A f into in time delta t this is what the moles of j would come in and go out and what about generation? Generation typically if you recall we denote it per unit volume of the volume of the reactor. So let us say the volume of the reactor is A delta z, A is the cross section area in time t and for time being I am just going to put q m j as the rate of generation of this species j.

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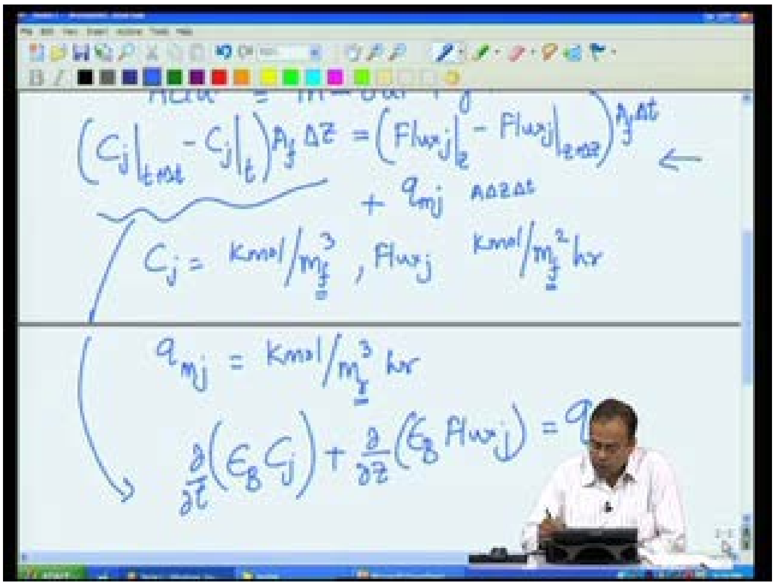

$$\left(C_j\big|_{t+\Delta t} - C_j\big|_{t}\right) A_f \Delta z = \left(Flux_j\big|_{z} - Flux_j\big|_{z+\Delta z}\right) A_f \Delta t \leftarrow$$

$$+\, q_{mj}\, A \Delta z \Delta t$$

$C_j = kmol/m_f^3$, $Flux_j$ $kmol/m_f^2\,hr$

$q_{mj} = kmol/m_r^3\,hr$

$$\frac{\partial}{\partial t}\left(\epsilon_B C_j\right) + \frac{\partial}{\partial z}\left(\epsilon_B Flux_j\right) = q$$

Now you may wonder, what this q m j is, we will for time being leave it at q m j and the reason for this will become clear, as we go on developing different types of models. So right now we will just say that q m j is the rate. So once again if we look at my C j it is let us saying kilo mole per meter cube of the fluid and these units are important to keep in mind. Because otherwise we would not have consistency of consistency of units for all the terms in our mass balance and we are likely to make some mistakes. Flux of j is again kilo mole per let us say per hour.

Again the fluid volume both these are per fluid volume and for that reason why we choose this will become clear q m j, we are going to call it kilo mole per reactor volume per hour and therefore, so this is per reactor volume and we multiplied it by reactor volume A delta z in our mass balance equation. So this is my mass balance equation. Now if I divide this by A delta z delta t and take a limit as delta z goes to zero delta t goes to zero that is converted difference equation into a differential equation we will get. For example, the first term over here the accumulation term will simplify to remember we are dividing by A delta z.

So A f by A that is my epsilon bed the fluid volume by the bed volume epsilon B C j dou dou t. So that will represent my accumulation term plus once again dou dou z of epsilon B into flux of j if I take this term on the other side and use appropriate unit equal to q m j is my is my energy balance. Now, what is my flux of j?

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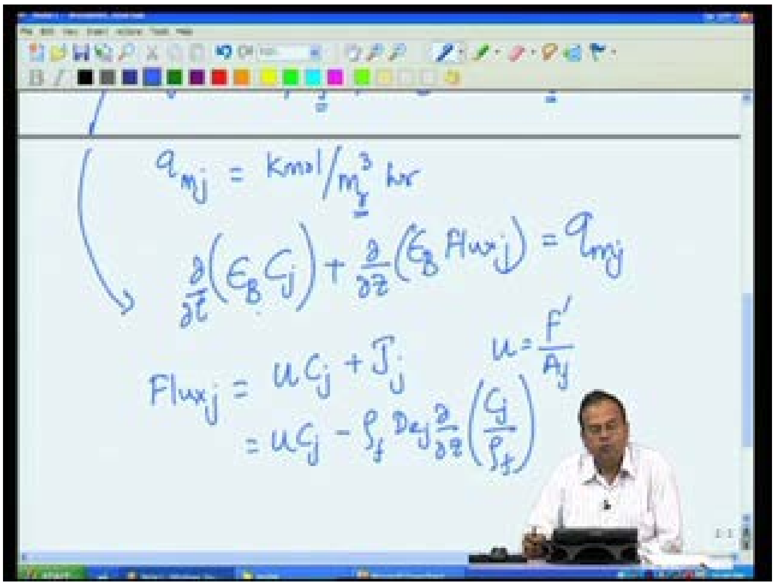

$$q_{mj} = kmol/m_{r}^{3}\,hr$$

$$\frac{\partial}{\partial t}(\epsilon_B C_j) + \frac{\partial}{\partial z}(\epsilon_B Flux_j) = q_{mj}$$

$$Flux_j = uC_j + J_j \qquad u = \frac{F'}{A_f}$$

$$= uC_j - \rho_f D_{ej}\frac{\partial}{\partial z}\left(\frac{C_j}{\rho_f}\right)$$

I can write my flux of j remember my flux of j two components u into C j plus diffusive flux, u is my interstitial velocity. So u is my fluid floret F prime divided by A f. So I can write this u into C j minus if I use my diffusive flux that gives me my fluid diffusive flux rather and this is convective flux. So these together give me my total flux. Now if we if we put all these things together we get our mass balance equation.

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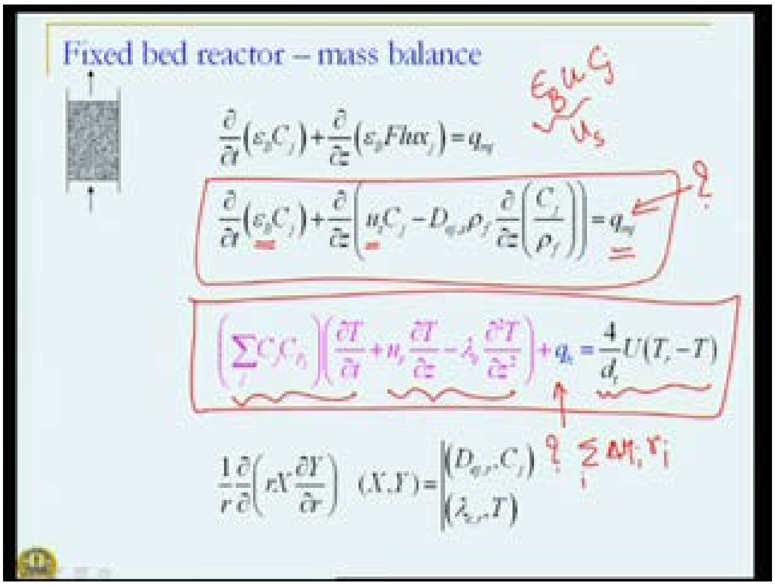

Fixed bed reactor – mass balance

$$\frac{\partial}{\partial t}(\varepsilon_B C_j) + \frac{\partial}{\partial z}(\varepsilon_B Flux_j) = q_{mj} \qquad \frac{\varepsilon_B u C_j}{u_s}$$

$$\boxed{\frac{\partial}{\partial t}(\varepsilon_B C_j) + \frac{\partial}{\partial z}\left(u_s C_j - D_{e,z}\rho_f \frac{\partial}{\partial z}\left(\frac{C_j}{\rho_f}\right)\right) = q_{mj}} \leftarrow ?$$

$$\boxed{\left(\sum_j C_j c_{pj}\right)\left(\frac{\partial T}{\partial t} + u_s \frac{\partial T}{\partial z} - \lambda_z \frac{\partial^2 T}{\partial z^2}\right) + q_h = \frac{4}{d_t}U(T_c - T)}$$

$$\frac{1}{r}\frac{\partial}{\partial r}\left(rX\frac{\partial Y}{\partial r}\right) \quad (X,Y) = \begin{vmatrix}(D_{e,r}, C_j)\\(\lambda_{e,r}, T)\end{vmatrix} \quad ? \ \sum_i \Delta H_i r_i$$

So that mass balance equation now takes form of this particular equation namely, which we just now just now derived denoting the flux, the accumulation and generation. Note here what we did from that particular equation to here is we multiplied epsilon B into interfacial area into C j and denoted this by superficial velocity so that is where superficial velocity. So that is where that u s comes in this is our standard diffusive flux equation and q m j is my mass balance. So this is my mass balance for fixed bed reactor. I have not yet specified what this q m j is.

Now if you recall this equation is exactly identical to identical to our tubular reactor mass balance equation that is if we go back to this equation. This equation and my fixed bed reactor is exactly identical except what I have done now is I have said we have this epsilon B factor because the entire bed cross section is not available for fluid to flow, only the fraction of it epsilon B is available so that is one change. Here because of that same effect entire fluid is not available for or the cross section is not available for flow. So we have velocity u s and then there this term was the rate of generation simply the kinetic rate.

But remember we have now transport phenomena within that are internal as well as external diffusion phenomena associated with the catalyst palette that is responsible for telling me what the rate of reaction is. So I have to now make suitable assumptions and put some values for that rate. But before we do that we will just now take it that our energy balance will also be similar to that for a tubular empty reactor with the exception that with the exception that this is now heat generation rate not necessarily the term which we had seen earlier summation delta i H i r i summed over all reaction rate that we will not be using over here.

But otherwise this is my accumulation term. This term represents my conduction as well as convective of flow energy transport and this denotes my energy added by external or surrounding fluid. So in that sense our mass balances are very similar to what happens for a tubular reactor. However there are certain differences and we will now look at what is we are still are silent on what is this q m j and q h.

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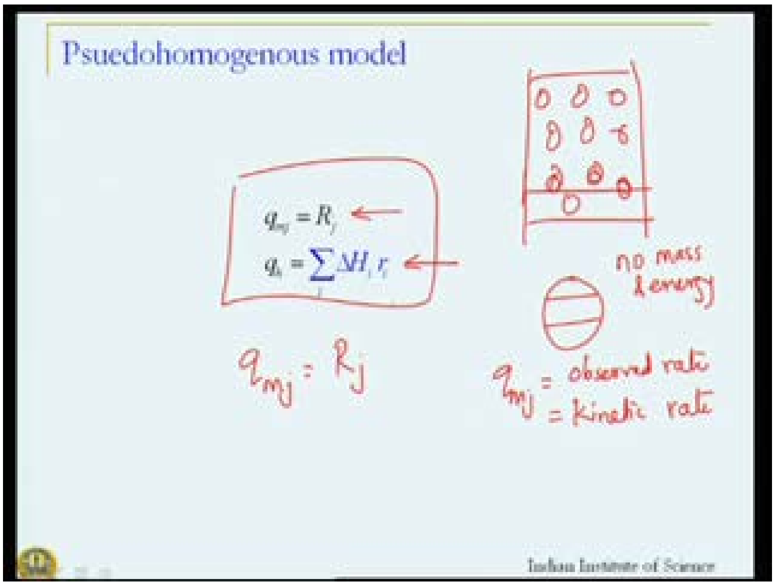

Psuedohomogenous model

$q_{m_j} = R_j$

$q_h = \sum_i \Delta H_i r_i$

$q_{m_j} = R_j$

no mass & energy

$q_{m_j}$ = observed rate = kinetic rate

How do we how do we define those? That is what we will now focus our attention on. Now let us say that we have our catalyst bed there are these catalyst particles catalyst particles. But let us take one such particle and if we say that the both mass and energy transport limitations are not present. So no mass and energy transport limitations which means what the concentrations inside are uniform temperatures are uniform in which case the reaction occurs at the same rate throughout the catalyst palette and since we are assuming all catalyst palette at a given cross section are identical, I can simply say my rate of mass transfer generation is nothing but the rate of reaction.

This is equivalent to saying actually from our earlier notation q m j is nothing but the observed rate and if there are no mass and energy transport limitation this is nothing but the kinetic rate. Therefore, q m j is my rate of reaction R j and q h again taking the same analogy is nothing but summation of delta H i r i. So what have we what have we now assumed? We have assumed that even though we have catalyst particles the diffusional and mass and energy transport limitations are not there. As a result we see that our mass balances with this particular kind of substitution will actually be exactly identical to that is q m j is R j this is nothing but H i r i will be exactly identical to our mass and energy balances for homogenous system.

Hence this assumption or this kind of modeling approach is referred to as pseudo homogenous model homogenous because the kinetic terms are same as homogenous model but pseudo because this is not a truly homogenous system, we know that there is a heterogeneous system but our observation is that there are no mass and energy transport limitations and therefore we completely overlook this aspect of transport limitation and get a model which is similar to pseudo homogenous model. So this kind of multiphase model is often refer to as pseudo homogenous models. But what if mass and energy transport limitations are really present in our present in our system.

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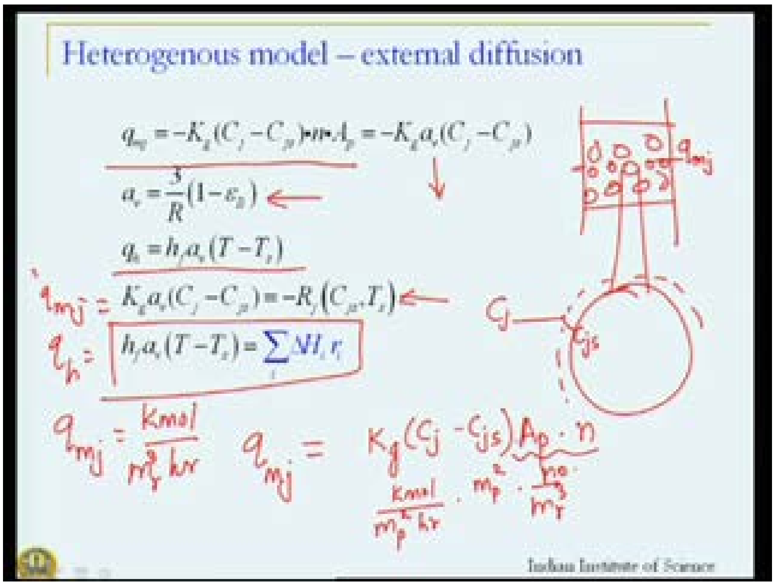

## Heterogenous model – external diffusion

$$q_{mj} = -K_g(C_j - C_{js})\, n A_p = -K_g a_v (C_j - C_{js})$$

$$a_v = \frac{3}{R}(1-\varepsilon_B) \leftarrow$$

$$q_h = h_f a_v (T - T_s)$$

$$q_{mj} = K_g a_v (C_j - C_{js}) = -R_j(C_{js}, T_s) \leftarrow$$

$$q_h = \boxed{h_f a_v (T - T_s) = \sum_i \Delta H_i r_i}$$

$$q_{mj} = \frac{kmol}{m_r^3\, hr} \qquad q_{mj} = \underset{\frac{kmol}{m_p^2\, hr}}{K_g(C_j - C_{js})} \underset{m_p^2}{A_p} \cdot \underset{\frac{no}{m_r^3}}{n}$$

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So let us consider that scenario so once again what we are saying is that we have this catalyst bed. Now if I look at one of this catalyst particle and let me start saying that first only external diffusion limitations are important. What we are looking for is q m j which is kilo mole per meter cube of reactor volume per hour. So what is the rate of this reaction? Now if you recall our discussion on external mass transfer limitations we said that there is thin film which surrounds this. So if this C j is my bulk concentration up to this point it is same as C j but then concentration decreases and concentration on the surface is C j s and the reaction rate must be equal to the mass transfer rate.

So what did we write for individual single particle we wrote that K g into C j minus C j s must be the rate of reaction or rate of change of j th species for this one particular catalyst. Now this rate is per unit catalyst surface area. So let us multiply this by the surface area of the catalyst so this one is kilo mole per catalyst surface area per hour. So let us multiply this by m p square but at a given cross section we do not have only single particle, we have n number of particles. So multiply this by number of particles per unit volume of the reactor. So number per m r cube will give me my required q m j.

Indeed this is my q m j that is at this cross section the particle or the species j will see is generation, which is equivalent to the mass transfer rate times A p times n. We can write A p into n as a v that is catalyst surface area per unit volume of the volume of the catalyst and if we assume spherical particle that a v works out to be 3 by R 1 minus epsilon B. Now what is this q m j or this mass transfer rate? This must be same as my reaction rate that is what we say that there is no accumulation on the surface of the catalyst. So whatever is coming because of mass transfer is same as the reaction rate.

So K v K g into a v into C j minus C j s must be equal to minus R j into C j s R j which is a function of surface concentration and temperature. What about energy balance we will do the same thing that is energy transported to the surface must be counter balanced by the heat the heat effect of the reaction and therefore we say that q h just as mass transfer q m j was given by this particular term q h is given by h f that is the heat transfer coefficient times a v that is the particle surface area per unit volume of the reactor multiplied by T minus T s, where T is the bulb temperature T s is the surface temperature and what this must be equal to this must be counter balanced by the energy effects in the in the reactor.

So this in fact gives us our required quantities in our generalized mass and energy balance equation. This under the condition that only external diffusion limits the rate of rate of reaction or what if internal diffusion is also there if internal diffusion is there.

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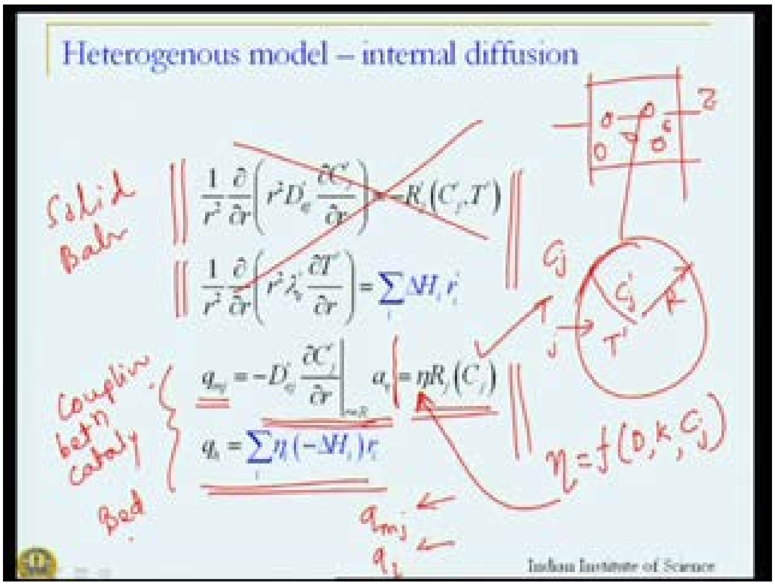

Heterogenous model – internal diffusion

$$\cancel{\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 D_e' \frac{\partial C_j'}{\partial r}\right) = -R_j(C_j', T')}$$

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \lambda_e' \frac{\partial T'}{\partial r}\right) = \sum_i \Delta H_i r_i'$$

$$q_{mj} = -D_{ej}' \left.\frac{\partial C_j'}{\partial r}\right|_{r=R} \qquad q_{mj} = \eta R_j(C_j)$$

$$q_h = \sum_i \eta_i(-\Delta H_i) r_i$$

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So let us go back so this is our bed. Let us say we are looking at some cross section this particular particle over here and now what we are what we are saying is that this particle let us say we do not have external diffusion but only internal diffusion so let us say that C j is my concentration over here. The concentration is going to decrease continuously so let us say C j prime is the concentration inside. Same is the case with my temperature T and T prime and what describes the diffusion and reaction in the catalyst palette this is my mass balance same as what we saw earlier. Energy balance again similar for single particle the only difference is my q m j now.

Now if you position yourself into this bed all that bed will experience is that there is a diffusive flux of species j at the surface. Because there is no reaction in the bulk liquid the reaction is only inside. So all that we will experience if we are in the bulk is that j is diffusing in the catalyst palette. So the mass transfer or rate of generation of j q m j must be this diffusive flux at radius of the catalyst palette R. This is what this is what for a single particle multiplied once again by the number of particles per unit volume of the area, this is what will give us what is the rate at which species j is changing in the bulk.

Now we also know from this mass balances and respective boundary condition we can write this whole thing as effectiveness factor that is nothing but my observed rate. Now but per unit volume of the reactor which we can write as effectiveness factor into the rate at the bulk conditions that is what the beauty of this effectiveness factor effectiveness factor is. Similarly for q h that is my energy balance when both internal mass and energy limitations are important.

So let me recap once again what we are saying is that we are writing now a heterogeneous model for a multiphase reactor. Why heterogeneous because we acknowledge that solids are distinct phase in our reactor. So we describe what is happening in the solid and then couple it to what is happening in the bed. So this is my solid phase balances and this is my coupling between the catalyst particle and the bed of the reactor or the reactor.

Why this coupling is where is it used this is my reactor equations reactor equations and these two quantities couple these reactor equations with my bed equations and that is why we initially choose to write q m j and q h as the rate of generation of species j in the bulk and rate of generation of energy q h in the bulk and then depending on how we visualize this processes to are taking place we define q m j and q h differently that is if we say that there are no mass and energy transport limitations then q m j and q h are simply reaction rates and rate of heat generation due to reaction.

If external diffusion is important then q m j is nothing but the rate of mass transfer from bulk to the surface of the catalyst which is the same as rate of reaction at the surface conditions and similarly for energy. If we assume that both energy and mass internal limitations are there internal transport limitations are there. Then we have to write separate balances for solid phase and couple them through these boundary conditions. I mentioned about beauty of effectiveness factor. Now just assume that if we use these balances these balances not the second part so that is where effectiveness factor is there if we just use this then for solving my reactor balance I have to solve these solid balances calculate these flux and plug it in.

But what if  a priori or independently calculated my effectiveness factor as a function of let us say diffusive characteristic reaction rate constants bulk conditions. If I had this knowledge a priori I could have substituted it over here and without solving this mass and energy balances I would have simply got my coupling that I required to solve my reactor balance and this is why this effectiveness factor approach is popular. Even though we have now fancy computers which can solve any kinds of equations for us, the elegance of this method still carries the D. So this is this is where the effectiveness factor which is almost fifty years old concept is still applicable and useful in todays scenario also.

So this is as far as developing the general mass and energy balance equations for our reactors both homogeneous and heterogeneous. We will talk about more of these reactor mass balances whenever we discuss specifically reactors such as fluidized bed reactors little later on. But before now let us let us now look at different types of reactors and their behavior. One of the important reactor behaviors is associated with non-isothermal a reactor that is reactors in which the temperature is not constant. If you recall my first lecture I had mentioned that when we study our undergraduate material we typically deal with isothermal reactors.

But isothermal reactors are only ideal. The real reactors are invariably non-isothermal why is that that is because reactions are either absorbed or release large amount of energy that is the heat of reaction depending on weather the reaction is endothermic or exothermic and secondly reaction rates are sensitive to fluctuations in temperature more than the fluctuations in concentration. Recall the concentration dependency can be linear or mildly linear second order and so on or a priori kind of kinetics. But the temperature dependency is exponential and so small increase in temperature causes their change of rate of reaction to be several orders of magnitude.

So that is why non-isothermal reactors are invariable. Now there are situations where for example, for exothermic reactions non-isothermal operation is a preferred mode of operation over isothermal reactor. The reason for this is that we have large amount of energy that is released by the reaction now what do we do with this energy. We can use this energy to increase the temperature of the reacting fluid so that you get high reaction rates. But we it comes to exothermic system as we will see shortly there is a dilemma because if we raise the temperature of the reacting system to a very high value where equilibrium conversion is adversely affected.

So if temperature is too high equilibrium is bad, if temperature is too low the kinetics is poor either way it is a lose it is no win situation. So better to make use of heat of reaction and operate the reactor in a non-isothermal manner, so that we can make use of the energy that is liberated to do certain things. What are those certain things? We will see in the future lectures. The main another reason why we should worry about isothermal non-isothermal operation is because invariably as the reactor size increases temperature control is difficult.

You may be able to control the temperature of a small test tube or a small beaker just by putting it in a thermostat but imagine doing that for a reactor which is hundreds of meter cube of volume, very challenging task and therefore operations are preferred as non-isothermal because control may not be possible. But more than that even if you are trying to do an isothermal operation the knowledge of non-isothermal behavior is extremely important to understand what if kind of scenarios.

What if my cooling fluid system cooling system completely fails I am running an exothermic reaction in an isothermal manner in a reactor but my cooling system fails, what will happen or my pump fails what will happen? So to understand what if kind of scenarios which eventually may lead to serious accidents or failures of the processes? We must know what the behavior of the non-isothermal reacting system is. So let us let us try to focus on the simple behavior or behavior of simple reacting systems.

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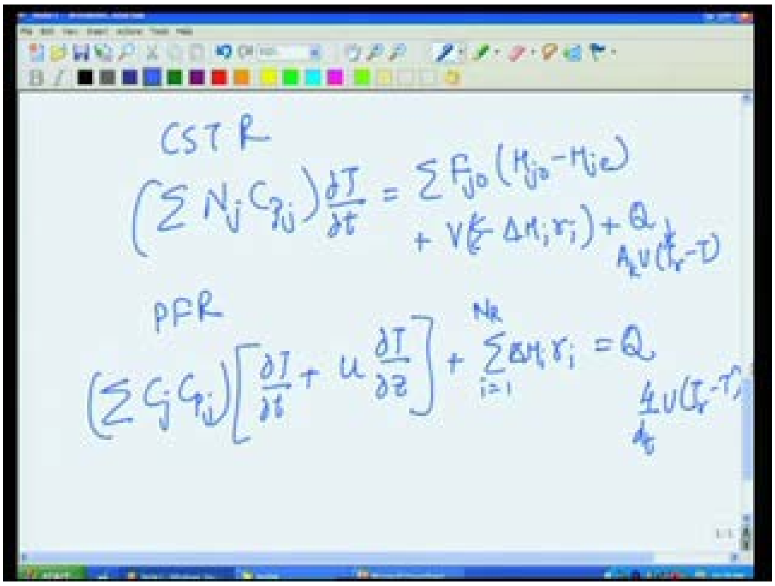

CSTR

$$\left(\sum N_j C_{p_j}\right)\frac{\partial T}{\partial t} = \sum F_{j0}\left(H_{j0} - H_{je}\right) + V\left(\sum -\Delta H_i r_i\right) + Q$$

$$A_x U (T_r - T)$$

PFR

$$\left(\sum C_j C_{p_j}\right)\left[\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial z}\right] + \sum_{i=1}^{N_R} \Delta H_i r_i = Q$$

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

Let us try to look at how this reactor will behave. So let us let us try to look at the non-isothermal behavior and before we do that let us rewrite our mass and energy balances only energy balances mass balances we already know. So let us say that for CSTR we wrote the energy balance as N j C p j dou T by dou t equal to summation F j zero H j zero that is enthalpy of stream coming in plus V minus delta H i summation H i r i into plus Q, Q which is A k into T r minus T so this is my mass or other energy balance. For my stirred tank reactor and for my plug flow reactor my energy balance is summation C j C p j into dou T by dou t accumulation term plus u convective transport plus equal to Q, where Q here is 4 by dt T r minus u into T r minus T so this is my stirred tank reactor equation, this is my plug flow reactor equation.

Let us first try to understand what is meant by operating a reactor in an isothermal manner when energy effects are energy effects are important. So when we want to operate the reactor in an isothermal manner isothermal manner then temperature is constant so we can put these accumulation terms to be accumulation terms to be zero. These terms to be zero and similarly, the term that is the convective term also to be zero and simply say that to maintain let us say for a for a stirred tank reactor at stationary or at constant temperature or isothermal reactor what is it that we require.

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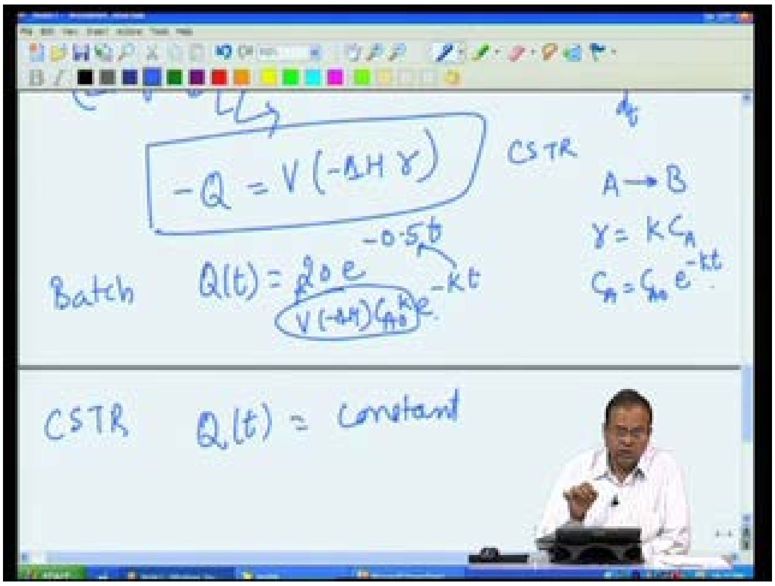

$$\boxed{-Q = V(-\Delta H r)}$$

CSTR

$A \to B$

$r = kC_A$

$C_A = C_{A0} e^{-kt}$

Batch $Q(t) = Q_0 e^{-0.5t}$

$V(-\Delta H) C_{A0} k e^{-kt}$

CSTR $Q(t) = \text{constant}$

So according to this energy balance minus Q must be which is which is our A k u into T minus T r must be same as from these particular balance V into minus delta H into r the rate of reaction. Because we are assuming let us say a batch reactor isothermal reactor so that so that we do not have a temperature of the let us say that we are looking at continuous system. But enthalpy in an out is same that is temperature is of the inlet is same as the temperature of the outlet, so we are maintaining that temperature. So what does it what does it take so for example, in CSTR this is what is required to maintain that temperature constant. What is it that is that is required in a batch reactor?

Let us say now for a batch reactor I am just going to assume my first order reactions. So let us say that we have reaction A going to B the rate of these reaction is K into C A, where K is a function of time and if we use we are going to use isothermal. So we know my concentration changes from my initial concentration in an exponential manner. So if I now take all this together that is concentration decreasing exponentially with time put it over here put it back into this I will get my heat of removal will be I am just putting some numbers it does not mean so much at this point.

But all I am trying to do is say that V minus delta H C A naught e raise to minus k t into k value. So for a batch reactor assuming that this is all constant that is that 20 value output and k value of arbitrary 0.5. It means that to operate a batch stirred tank reactor in an isothermal manner. I have to remove energy in an exponential manner why because the rate of reaction for a first order system concentration changes decreases exponentially. So rate will decrease exponentially so my energy removal also has to be exponential.

What if we are operating this reactor as a stirred tank reactor continuous process? In a continuous process V is constant delta H is constant rate is constant. So it would mean that Q of t is a constant that means for a stirred tank reactor I have to keep on removing the energy or supply the energy depending on weather it is a endothermic or exothermic reaction at a constant rate. For a batch process it has to change exponentially with time. What happens in a plug flow reactor? Plug flow reactor also equation is same so what will happen for a plug flow reactor.

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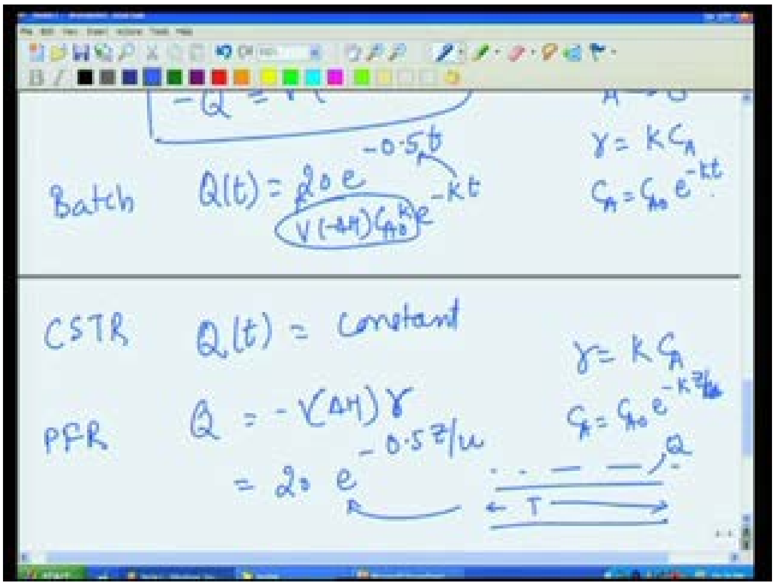

For plug flow reactor again I will say my Q which is if we go back over there that is now all this term are zero so Q is this. So if my Q which is minus delta H into r, r once again K into C A but for a tubular reactor C A is C A zero e raise to minus k z by l the length of the length of the reactor z by u z by u the velocity it is actually K into residence time. Or in other words this now will be some number I want to just put some numbers again numbers do not mean but what it means is that if I want to maintain the temperature uniform through the entire reactor bed I have to remove energy Q at a rate which changes along the length of the reactor.

Why because for a tubular reactor concentration decreases exponentially along the length of the reactor. So the rate of reaction will decrease exponentially along the length of the reactor and therefore, the rate of generation of energy will change exponentially along the length of the reactor and therefore the heat to be added or removed to maintain the temperature constant will have to also change along the length of the length of the reactor. Not an easy thing to do. How do you how do you achieve that? You will either have to change what the reference temperature along the length of the reactor not an easy task to do.

You will have to do something so that the rate of the rate of heat added or removed is exponential. So as I said maintaining isothermal conditions even though easier said on paper is very difficult in practice particularly for tubular reactor. How do you do that?

Because you have to change your heating or cooling rate along the length of the length of the reactor.

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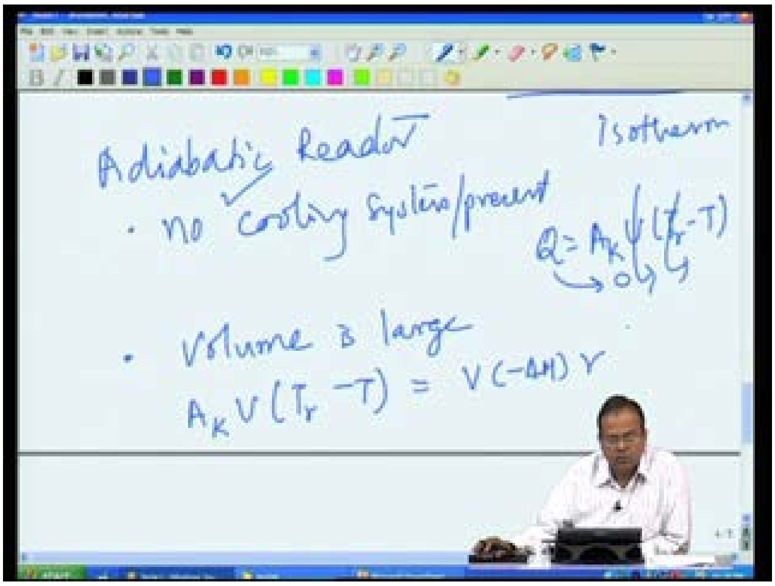

Adiabatic Reactor

Isotherm

- no cooling system/present

$Q = A_k U (T_r - T)$

$\rightarrow 0, 0, 0$

- Volume is large

$A_K V (T_r - T) = V(-\Delta H) r$

Now isothermal is one end of the spectrum. What if I want to do these reactions in an adiabatic manner? So what is a adiabatic reactor? Adiabatic reactor is a one in which there is no heat added or removed from the system. So isothermal operation and the other extreme is adiabatic reactor, isothermal operation I am going to maintain the temperature constant whether it is possible or not is a different story. But I that is my aim what is adiabatic reactor adiabatic reactor is a one where you do not have heat added or heat removed from the system.

Now where do we come across such situations? One case where adiabatic reactor may actually be operating is when there is no coolant or no cooling or heating system is present no cooling or heating system is present. Now if you just to keep our Q is A k u into T r minus T. So if there is no T r or the heat transfer coefficient of the material is very poor Q is likely to be zero so that is that is one such scenario. Now another scenario is what happens when volume is large. Now going back to our isothermal operation we said that A k u into T r minus T is v into minus delta H into r. I am talking about a stirred tank reactor similar thing can be said about other reactor.

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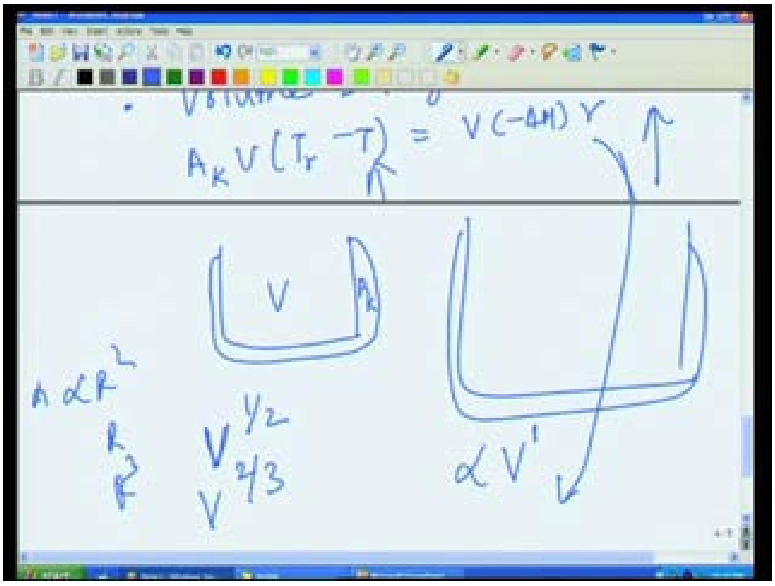

So let us say that this is my reactor this is my volume and this is what I am using to cool it. So A k is the area of this, now I increase my volume. I increase my volume what happens in my reactor system. My generation rate my generation rate over here is proportional to volume raised to power one but what about A k my heat removal rate. My heat removal rate if the reactor is cylindrical or tubular in nature. It will be V by half if it is spherical two-third and so on. Why because your area will be proportional to either R square or R or R cube depending on whether you have which kind of reactor.

So what we what we will have is that as our size increases our heat generation will increase V raise to one but our heat removal rate will only increase as either square root or two-thirds of V and so on. So what will happen? As we go on increasing the reactor sizes our cooling rate will be far lower compare to our heat generation rate leading to a situation where heat removal is practically negligible consider compare to heat generation. Another scenario of another scenario where adiabatic operation becomes important and a third case as I had said earlier is the what if kind of scenario what if I want to check weather my reactor isothermal operation fails isothermal operation fail means there is no heat removal or addition to the system.

What will happen to my reactor? So that is another aspect where my adiabatic operation will be important. So we will stop for this session and in the next session we will look at how does the adiabatic operations actually what happens when we have an adiabatic operation and how do we how do we relate the temperature concentration changes and so on. So in todays session what we sincerely saw was how do we develop mass and energy balances for heterogeneous reactors in particular for fixed bed reactors which are which are one of the most dominant kinds of reactors used in the industry. We also saw the importance of non-isothermal operation and how we how do we try do to we started actually the discussion on design of non-isothermal reactor systems, the details will be in the sessions to follow. Thank you.