Mass, Momentum and Energy Balances in Engineering Analysis

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Lecture – 29
Microscpic Balance – VI

Welcome we have seen how to model a double pipe heat exchanger, and we have written the model equations and we have understood that how a heat exchanger works and what are the various types of flow configurations possible in a double pipe heat exchanger. Now, we shall be now going ahead with the same problem as I told you in the last lecture that, a given model equation or model will be complete only when we specify the initial condition and the boundary conditions ok.

So, now we are going to tell you that, how to write the initial condition boundary condition for this kind of model equations.

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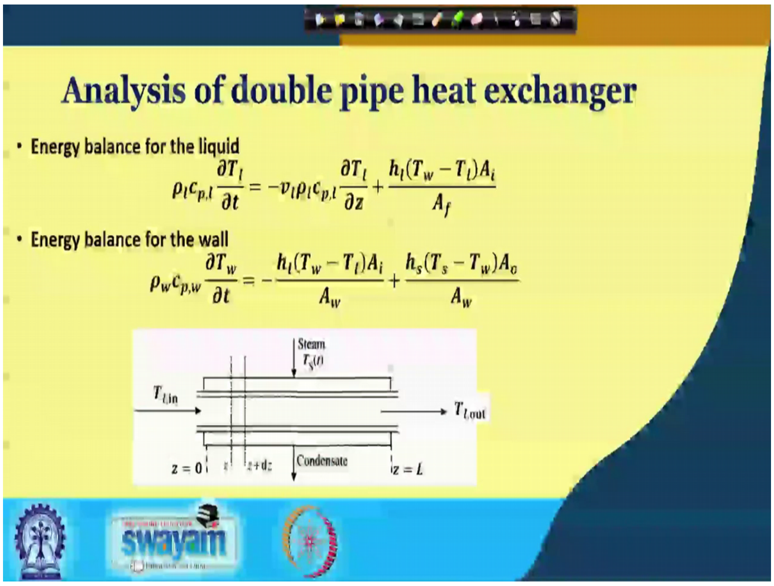

Analysis of double pipe heat exchanger

- Energy balance for the liquid

$$\rho_l c_{p,l}\frac{\partial T_l}{\partial t} = -v_l \rho_l c_{p,l}\frac{\partial T_l}{\partial z} + \frac{h_l(T_w - T_l)A_i}{A_f}$$

- Energy balance for the wall

$$\rho_w c_{p,w}\frac{\partial T_w}{\partial t} = -\frac{h_l(T_w - T_l)A_i}{A_w} + \frac{h_s(T_s - T_w)A_o}{A_w}$$

So, first let us recapitulate what we derived earlier. So, these are the 2 equations we wrote, one for the liquid and another for the wall of the inner tube ok. Now we is a starting point of our going further with the initial and boundary conditions.

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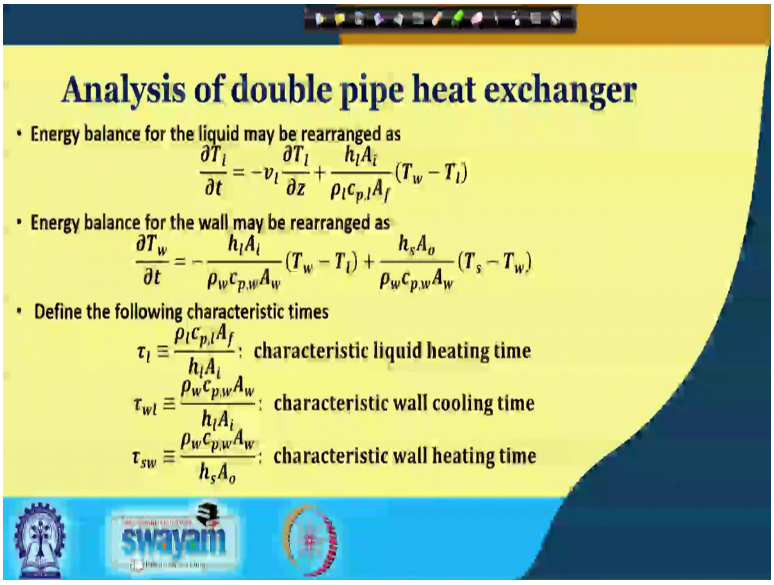

Analysis of double pipe heat exchanger

- Energy balance for the liquid may be rearranged as

$$\frac{\partial T_l}{\partial t} = -v_l \frac{\partial T_l}{\partial z} + \frac{h_l A_i}{\rho_l c_{p,l} A_f}(T_w - T_l)$$

- Energy balance for the wall may be rearranged as

$$\frac{\partial T_w}{\partial t} = -\frac{h_l A_i}{\rho_w c_{p,w} A_w}(T_w - T_l) + \frac{h_s A_o}{\rho_w c_{p,w} A_w}(T_s - T_w)$$

- Define the following characteristic times

$\tau_l \equiv \frac{\rho_l c_{p,l} A_f}{h_l A_i}$: characteristic liquid heating time

$\tau_{wl} \equiv \frac{\rho_w c_{p,w} A_w}{h_l A_i}$: characteristic wall cooling time

$\tau_{sw} \equiv \frac{\rho_w c_{p,w} A_w}{h_s A_o}$: characteristic wall heating time

So, before we go for the initial boundary conditions, let us do some rearrangement of the 2 equations. And what we have done that you can see that we have written this, but on the left hand side we have only the variation of the temperature with time and rest of the variables we have taken the right hand side.

And now what we see that, if you look at this particular term you can see that this particular term has a dimension that is the inverse of the time ok. So, that is why in this whole 2 equations we find that, this particular it means this term or that this particular term will have the dimension of inverse of time. So, we are finding that we have different types of characteristics times. So, here we are defining the various types of characteristics time and here this is 1 tau l 1 is tau w l and 1 is tau s w.

What is tau l? This is the characteristic liquid heating time; that means, you can see that this is the numerator is giving us the heat content of the liquid, and this is the heat that is been coming to heat up the liquid from the wall. So, we can see that the higher this time ; that means, it will take longer time for the liquid to get heated up ok. So, this is the characteristic time for the wall cooling time. When wall cooling because this is involving this numerator is again the heat content of the wall, but now in this case this is hl; that means, the how much heat is going from the wall to the liquid and this is tending to cool down the wall ok.

So, that is why we are calling it characteristic wall cooling time. And another one is coming like this here, you can see again the numerator is same as this one that is a heat content of the wall this, but here you see that is difference right. This is the one that is the convective heat transfer coefficient in the steam, and this is trying to heat up the wall by transferring the heat from the steam to the wall. So, we are calling it characteristic wall heating sign.

So, these are the three types of time dimension times involved in this particular process and how does it help? It helps that you can without really going into the values of each of these; we can change these values over all values and take that how the various types of heat transfers would be affecting the overall process.

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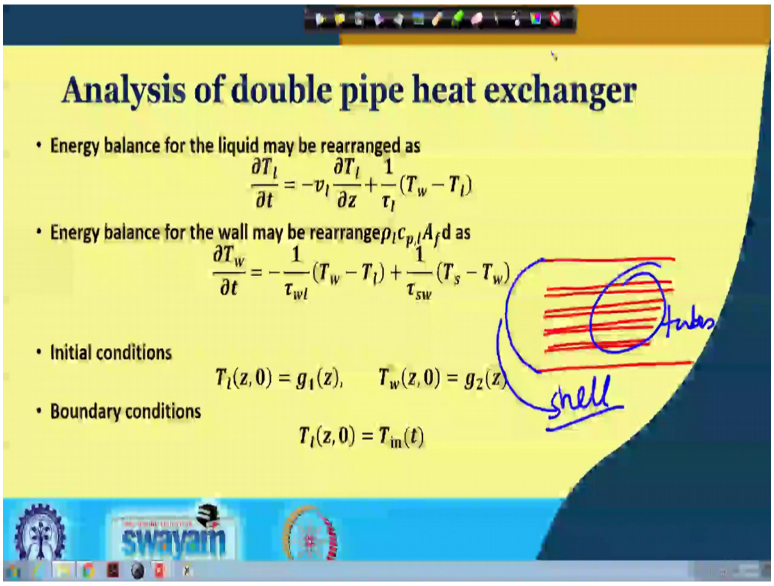

Analysis of double pipe heat exchanger

- Energy balance for the liquid may be rearranged as

$$\frac{\partial T_l}{\partial t} = -v_l \frac{\partial T_l}{\partial z} + \frac{1}{\tau_l}(T_w - T_l)$$

- Energy balance for the wall may be rearrange$\rho_l c_{p,l} A_f$d as

$$\frac{\partial T_w}{\partial t} = -\frac{1}{\tau_{wl}}(T_w - T_l) + \frac{1}{\tau_{sw}}(T_s - T_w)$$

- Initial conditions

$$T_l(z,0) = g_1(z), \qquad T_w(z,0) = g_2(z)$$

- Boundary conditions

$$T_l(z,0) = T_{\text{in}}(t)$$

Now, with this kind of rearrangement what we find that, we have these 2 equations and you have seen that here we have this particular term is replaced by 1 by tau l, this is 1 by tau T w and this is 1 by tau is w.

So, you can also write or convert the given model equation in this term and this way you can see that how elegantly you can represent the model equations and this is done mainly at times in various other processes ok. So, this is I have just shown you, how you can do this kind of rearrangements and define some new kind variables to make the equations more compact and sometimes more elegant.

Now, coming to the initial condition and boundary conditions; now you see that the initial condition means at time t equal to 0 ok. Now at time t equal to 0 we miss and we can say that the liquid temperature may have some kind of distribution. This g 1 shows some kind of distribution at the time t equal to 0. It need not be constant it may have a distribution; that means, there could the liquid may have different temperatures along the z direction.

Similarly, the solid that the wall of the container, the solid may also have a distribution of temperature along the length along the z direction it need not be constant ok. So, that is why we are putting in general g 1 z and g 2 z. Next to the boundary conditions; that means, at the inlet and at the outlet. As we have seen that the in case of the wall we do not need any boundary condition because in case of the wall we do not have any derivative with respect to z, but in case of liquid we have a derivative with respect to z.

So, as we learnt earlier that because we have this spatial derivative so, we need a special condition that is the boundary condition. So, for the liquid we are saying that the inlet of the liquid we are specifying some temperature t in ok. And now also you see that this inlet temperature may be a function of time it need not be constant it may also vary with time ok. But there is nothing no boundary condition for the solid because in the solid there is no derivative with respect to the z.

So, this is how we have completely modeled this particular double pipe heat exchanger. You can extend this same analysis for various other types of heat exchangers like shell and tube heat exchangers. Shell and tube heat exchanger is nothing, but you can imagine that shell and tube heat exchanger is a multiple this double pipe heat exchangers. It looks like this that you have a shell that is a body a cynical body and you can see that in the there are many many tubes here not one, there are many tubes here ok.

So, there are bunch of tubes and again this bunch of tools may be added in different manners ok. So, these are the these are the tubes these are the tubes and this thing you can call this is the shell ok. So, you this similar kind of a configurations flow configurations can be there parallel configuration co the co current counter current cross flow, all these kind of considerations may also be there in this shell and tube. So, these are the simple and very simplistic heat exchangers there are many other complexity exchangers also in the industries.

But whatever they may be the if you can identify the control volumes properly, you can write the model equations very easily and also can write the initial and boundary conditions.

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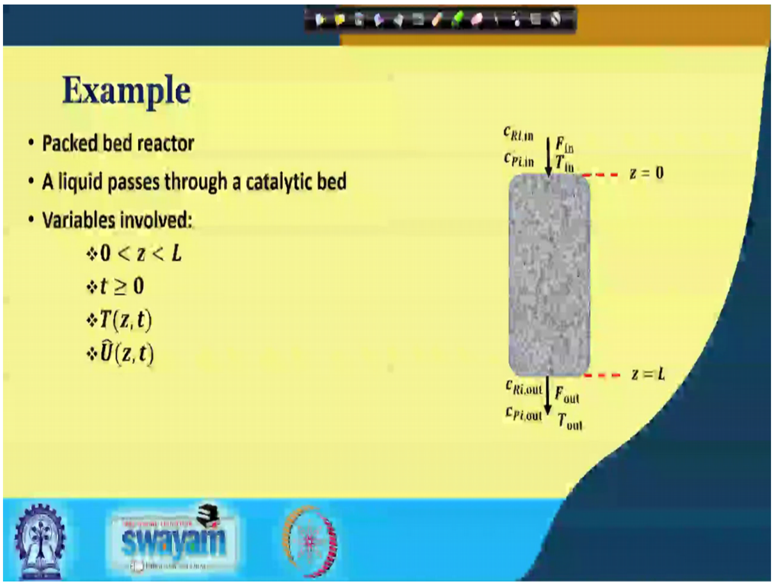

Example

- Packed bed reactor
- A liquid passes through a catalytic bed
- Variables involved:
  - ❖ $0 < z < L$
  - ❖ $t \geq 0$
  - ❖ $T(z,t)$
  - ❖ $\hat{U}(z,t)$

Now, let us move on to a different type of problem. Here we have a problem which is talking about a packed bed reactor. Now these packed bed reactors are used very often in the chemical industries and what is the meaning of packed bed means that, we had a column which is filled up with some packing. And packing has different purple such different purpose; one purpose is this the packings offer some surface area for the contact of the fluids.

Suppose we have a liquid and a gas. So, we want that these 2 things should get in touch contact with each other properly. So, we put this packing so, that these on the packing surface the liquid and gas will get contacted properly ok. And if there is no packing what will happen? These 2 fluids will flow out of the reactor very quickly and they will not be able to contact each other properly ok.

So; that means, we trying to enhance the order increase the contact time between the 2 fluids. Another purpose in case of reactors is this, that the packing itself are the catalysts. So, when the particular fluid is flowing through the packed bed, then these catalysts are helping in the performing that reactions ok. So, here you can see the packed bed reactor means that, the bed is filled with catalyst packing and in this a particular fluid is flowing through the bed and it is getting dispersed within this particular bed, and the reaction is taking place and we are getting some product and which is coming out.

Now, here you can see that the reaction R is signifying the reactant and P is the product and we are putting some kind of either component. Now here we are putting in and we are putting out over here to signify their inlet composition and the outlet composition. Now you see that now it may whenever the reactants are going inside the reactor and coming out, it is not that there will be 100 percent conversion some of the reactants will be remain going out without any reaction without any conversion ok.

And we will be having the flow in and flow out, now this flow in and flow out maybe if the moles are changing then we will find that the inlet flow rate is a different from the outlet flow rate. Even though the overall mass will be conserved, but if you go over the species by species, you will find the species flow rates are changing ok. And again due to the reaction we will find that there will be some temperature change because generally the reactions are either in; so, thermic or endothermic means inter atomic means the heat will be liberated during the reaction and endothermic means the heat will be absorbed during the reaction.

So, in case of exothermic reactions we find that the fluid will tend to heat up; in case of endothermic reaction we will find that the heat the fluid will tend to cool down. So, that is why you will find that there will be a difference in the temperatures between the inlet and outlet of the reactor. And in this case we are doing that we are designating the inlet as z. So, these are z direction. So, this is z equal to 0 and the height of the reactor is taken to be L. So, we are going what is z equal to L. And the variables involved are z as I total z under temperate time, time is more than equal to 0; that means, as I explained to the earlier lecture that the moment the fluid is introduced into the reactor is taken to be the time t equal to 0 ok.

And then we have the temperature of the fluid and that is a function of the z and t, and this is the heat content of the fluid that is also function of z and t.

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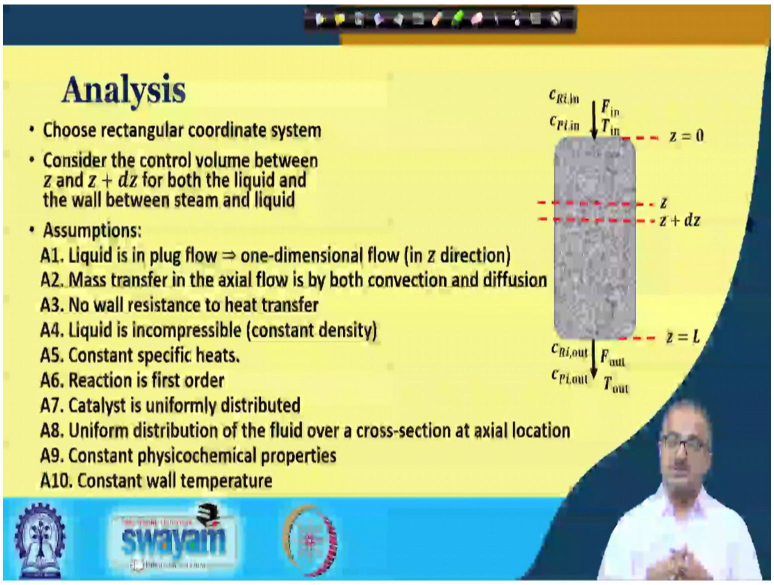

Analysis

- Choose rectangular coordinate system
- Consider the control volume between z and $z + dz$ for both the liquid and the wall between steam and liquid
- Assumptions:
  A1. Liquid is in plug flow ⇒ one-dimensional flow (in z direction)
  A2. Mass transfer in the axial flow is by both convection and diffusion
  A3. No wall resistance to heat transfer
  A4. Liquid is incompressible (constant density)
  A5. Constant specific heats.
  A6. Reaction is first order
  A7. Catalyst is uniformly distributed
  A8. Uniform distribution of the fluid over a cross-section at axial location
  A9. Constant physicochemical properties
  A10. Constant wall temperature

Now, even though the reactor is cylindrical, again we are assuming that there is a proper mixing along the radial direction and it is the axisymmetric process. So, in that case we are having only the variation the z direction that is axial direction. So, that is how we can adopt a rectangular coordinate system. And again we are taking a small element within this particular bed and this is this element is of height d z.

So, this element is situated at a distance z arbitrary is distance z from the inlet, and this is the other it is confined within this z and z plus dz domain ok. And now we are making any assumptions, now the liquid is in we are considering that the fluid is liquid. So, liquid is in plug flow. Now whenever we have liquid, we will generally put it from the top because the liquid tends to go down due to gravity. If the reactant is gas then you put it rather from the bottom because due to buoyancy, it will tend to move up ok.

So, if we follow this natural the tendency of the flow of the fluids what we do? We save; we save on the pumping power if we want to push a liquid from the bottom to top we would be needing a pump to push it up. Similarly if you want to put a gas to the top, then again we need some compress the gas to push it down ok. So, that is we are going against the nature. So, in general we try to follow their natural tendency of flow, and that is why this particular thing in this case we say that they say liquid reactant which is flowing down the reactor.

So, its the plug flow plug in means, that there is a complete mixing in the radial direction. So, there is only change the velocity is changing only in the axial direction. So, this is one dimensional flow in the z direction. Then mass transfer in the axial flow is both by convection and diffusion; that means, they provide diffusion because there will be a gradient of concentration as on the axial direction and due to this gradient, there will be a diffusive mass transfer. On the other hand due to the flow of the liquid there will be a convective mass transfer.

So, we are considering both the convective mass transfer and the diffusive mass transfer for knowing the change in the concentration of the various species involved. We are assuming that there is no wall resistance to heat transfer ok; that means, wall of the container is again having a very high thermal conductivity. So, it is not offering resistance to the heat transfer. So, the wall will be having in single temperature at any axial position. Liquid is incompressible that is it is having a constant density and this is a very usual assumption we make because the liquid density does not change significantly over a wide range of temperatures.

Then we have constant specific heats for the liquid and the reaction is taken to be a first order. Now it is not mandatory that you have to assume it to be first order, it can be any order of reaction. So, this is just for sake of illustration we are assuming that it is of the first order reaction. Now what is order of reaction and all this, I will not go to detail of this this will can be a learnt in a separate course on the reaction kinetics and this order is defined generally in for the elementary reactions ok.

So, without going to those details are not necessary as far as to understand these balanced equations. So, I am not going into detail of those fundamentals. We assume that the catalyst is uniformly distributed what it means is this? That the liquid is assumed to have a means uniform distribution over the cross section; however, to understand that in practice the liquid distribution is hardly uniform mean, we often we find there are channels or preferred path by the liquid whenever it flows through a packed bed ok.

And due to this what happens that, we find that some of the regions in the packed bed are being utilized for the reaction and some of the regions are what we call dry regions which do not see the liquid. So, that we find that there is a preferential flow of the liquid which causes say dry region and a wet region in the packed bed and that reduces the efficacy of the overall process.

However for the sake of simplicity, we are assuming that the liquid is getting distributed uniformly and the catalysts are also distributed uniformly so, that the weight voidage is constant. What is voidage? Voidage you know that whenever you are packing the bed what is happening? There are many many hollow mid means void spaces within the bed ok. And voidage is the ratio of void volume to the total volume of the bed. And when we are saying that the catalyst is only from the distributed we are easy assuming that the voidage of the bed is constant. And then we are assuming that constant physical chemical properties and constant wall temperature ok.

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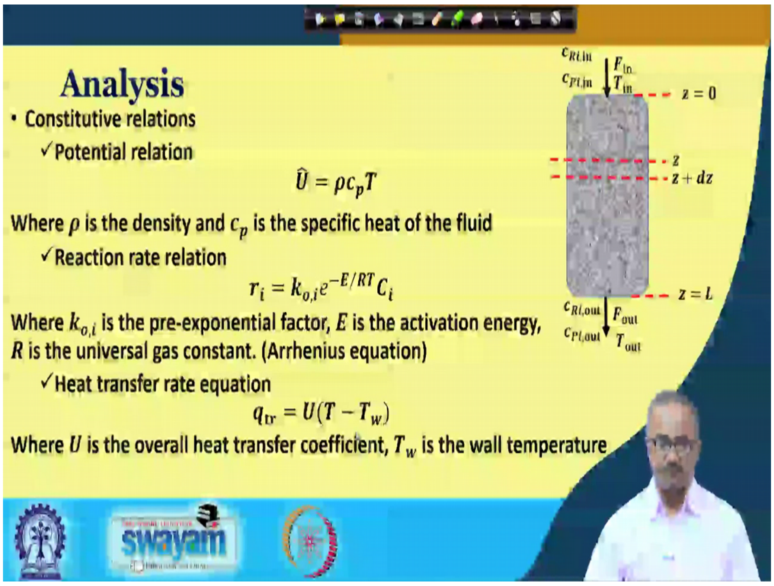

Analysis

- Constitutive relations
  - ✓Potential relation

$$\hat{U} = \rho c_p T$$

Where ρ is the density and c_p is the specific heat of the fluid

  - ✓Reaction rate relation

$$r_i = k_{o,i} e^{-E/RT} C_i$$

Where $k_{o,i}$ is the pre-exponential factor, E is the activation energy, R is the universal gas constant. (Arrhenius equation)

  - ✓Heat transfer rate equation

$$q_{tr} = U(T - T_w)$$

Where U is the overall heat transfer coefficient, T_w is the wall temperature

So, these are the other assumptions we are making. Now, coming to the mass balance; now, in this case because we are going to find out the distribution of the components ok. So, we are going with the mass balance. So, here we write the mass balance here. So, you can easily see that this is the accumulation term this is the diffusive term this is the convective term and this is the source term and the source term is generated due to the reaction if there is no reaction then there would be no source term.

So, you can understand the significance of each of the terms in this particular balance equation and this can be easily deduced from the Navier-Stokes equation. So, here we have the F is the flow rate, ri is the reaction rate of i th species d is the diffusion coefficient or what we call the diffusivity. Now as we said that the temperatures temperature at the inlet and the outlet are not remaining the same. So, we have to also write the energy balance equation and this we are writing here then again this is this term is the accumulation term ok.

This is causing the change in the temperature of the liquid and this is the diffusive term or the conductive term, here is the thermal diffusivity and this is the convective term this is the term which is a source term this is the heat generated due to the reaction is may be ultrasonic means positive generation endothermic means negative generation that is the heat absorption ok.

Whatever it is, with the proper sign of this delta h we can account for this if exothermic or endothermic reactions. And this particular thing is showing the heat transfer from the fluid to the atmosphere; that means, if we assume that the fluid is having a higher temperature than atmosphere, then if the heat will go out from the fluid to the outside. Now if we have an insulation; that means, insulation will say that we are having a 0 heat leak from the liquid to the outside, then in that case it will be an adiabatic situation and it is adiabatic then naturally this particular term will be taken to 0.

So, this particular term is a general term which can account for either adiabatic or isothermal or any other situation between adiabatic and isothermal. Now this particular new term we can write replace in terms of the density, specific heat and temperature of the fluid and here the reaction term may be given in terms of the Arrhenius equation. So, this is the Arrhenius equation in this you find that the system pre exponential factor, this E is the activation energy, this T is the temperature R is the universal gas constant.

So, this is how we can represent the reaction rate ok. And this activation energy is as such you do not need to know how it is coming it is the valid its value will be available in the literature in some books or some charts. Only thing is this to understand what is it? It signifies that how much energy it a particular or substance would need to cause the reaction because generally a whenever you are trying to cause any reaction, it has to be have enough energy to break the barrier to good for to the product side ok.

And this activation energy is signifying that energy barrier a reactant has to overcome to form the product. So, that is the significance of the active energy and the heat transfer rate is given by this particular equation, this is the overall heat transfer coefficient which includes the resistances on the liquid side within the wall of the tube or the column and in the outside ok. So, these resistances are clubbed together and they are put in terms of the overall heat transfer coefficient. Please mind remember that overall heat transfer coefficient is inversely proportional to the heat transfer resistance ok.

So, and here we have the wall temperature and we are assuming as if the wall temperature is at the outside temperature with this assumption we are writing this particular equation.

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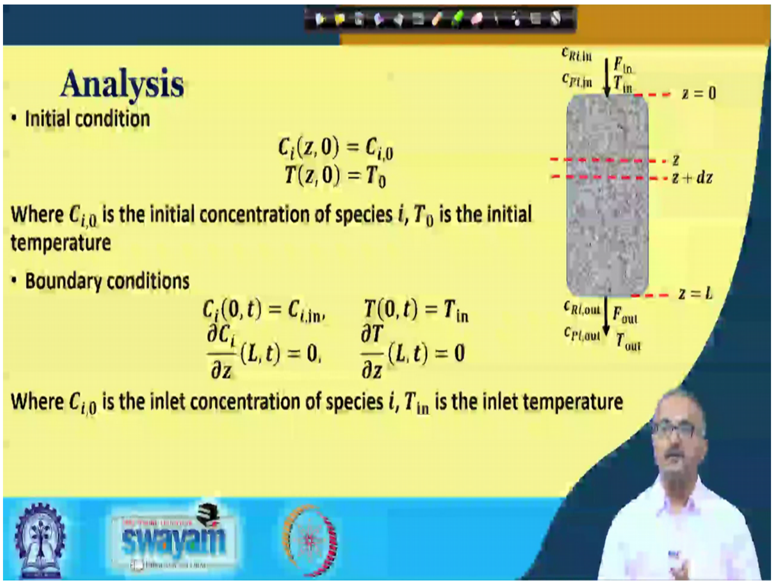

Analysis

- Initial condition

$$C_i(z,0) = C_{i,0}$$
$$T(z,0) = T_0$$

Where $C_{i,0}$ is the initial concentration of species i, T_0 is the initial temperature

- Boundary conditions

$$C_i(0,t) = C_{i,\text{in}}, \quad T(0,t) = T_{\text{in}}$$
$$\frac{\partial C_i}{\partial z}(L,t) = 0, \quad \frac{\partial T}{\partial z}(L,t) = 0$$

Where $C_{i,0}$ is the inlet concentration of species i, T_{in} is the inlet temperature

Now, again we go for the initial condition and the boundary conditions. In the initial condition; that means, at T equal to 0 we may specify some value of the i th component over the concentration and we can also specify the value of the temperature at the initial condition ok.

And so, the boundary condition what we can specify? These we can specify the actual concentration of the particular species ok. Now this is; that means, it is a reach that time condition type boundaries of type 1 similarly it deletes that condition for the temperature also. On the other hand at the outlet we do not make an delete that condition here we make a Norman boundary condition. Here we say that because it is not given to us what constants it come out ok.

So, we are saying that the flux at this outlet there is no flux of this particular thing, it is coming to a uniform as if it is coming to a uniform concentration at the outlet ok. And similarly we are also assuming that there is no heat flux at the outlet. Now understand these are some typical boundary conditions I have showed you, it need not be 0 here it may be if finite value or it may be a function of temperature of a time also. Similarly this need not be 0 it may have some non-zero value or a value which is varying with time.

So, these are take all these initial conditions, boundary conditions as some typical way of specifications, but not the absolute way of specification ok. So, we have to be very very careful you have to study the particular process properly before you start specifying the initial condition and the boundary conditions ok.

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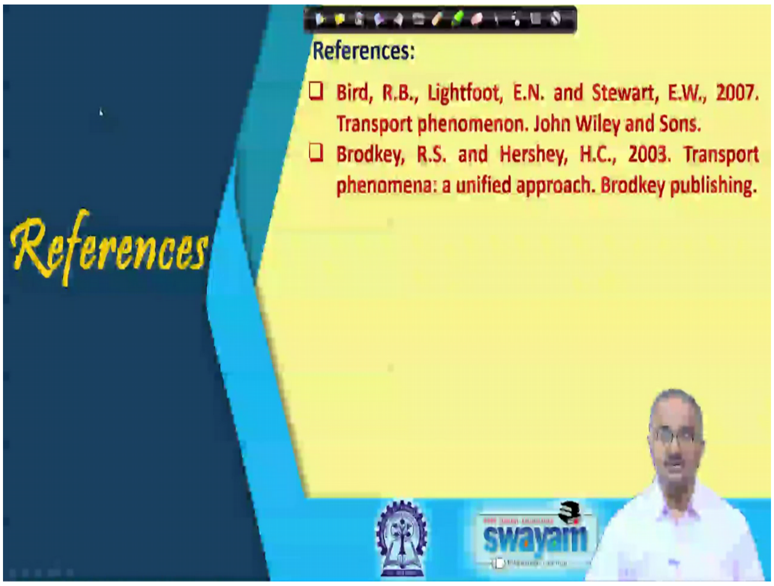

References

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- ☐ Brodkey, R.S. and Hershey, H.C., 2003. Transport phenomena: a unified approach. Brodkey publishing.

So, these are the references which you can consult to know more about the modeling of the various processes.

Thank you.