Transport Phenomena.

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Lecture-34.

Shell Heat Balance.

So the analysis that we are going to see in this class is about a reaction, it could be an exothermic reaction or an endothermic reaction which is taking place in a fixed bed reactor. And it is a catalytic reaction, so the reactants would enter the fixed bed reactor and then reaction would take place due to, in presence of the catalysts and the products will leave. And if it is an exothermic or endothermic reaction, then the temperature is going to be a function of the axial position.

So for example if it is an exothermic reaction, then as we move into the fixed bed reactor, the temperature of the reactant product mixture will progressively increase. And in order to give it a general flavour, it has been assumed that at the beginning and at the end of the reactor we also have a identical reactor attached to it. But these 2 reactors will not contain any catalyst particle. However these reactors are filled up with inert particles of the same size, same porosity, same arrangements as those of the catalyst particles in the actual fixed bed reactor.

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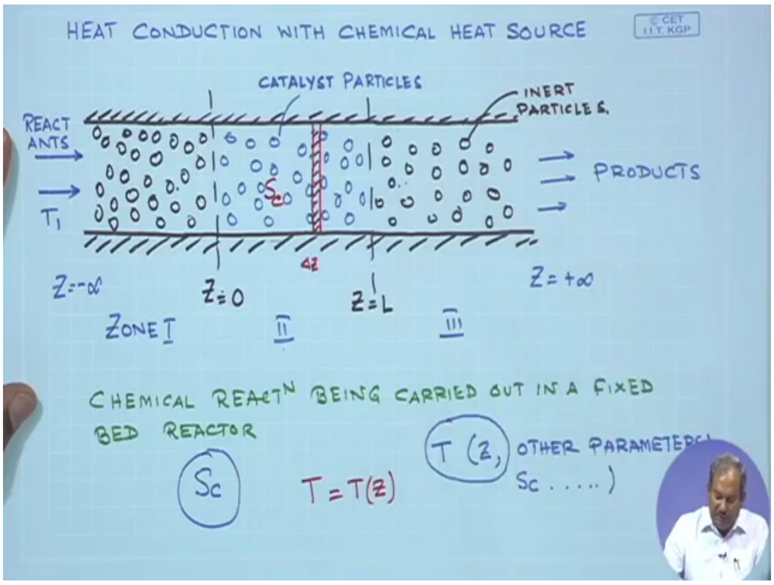

So the figure that we would use to solve the problem is that we have this catalyst bed reactors in which the blue ones are the catalyst particles, so the reactor starts at Z equal to 0 and up to a length of Z equal is L, the reactor is filled with catalyst particles and then from L onwards, we have certain length, a considerable length of the reactor in which inert particles of the same size, type, porosity, etc. of the catalyst particles are packed in here.

Similarly prior to Z equal to, prior to the location of Z equal to 0, all the way up to Z equal to minus infinity, mathematically speaking, that means whatever the large length, there would be another portion of the reactor in which all these particles, same, same size as those of the catalyst particles, same arrangement and so on, these are all inert particles. So we have a reaction that is taking place from Z equal to 0 to Z equals L and the reactants come through a section of the reactor in which no reaction takes place and then once the reaction zone is over, the products would travel through similar reactor but without any reaction and go out of the reacting system.

So we will assume that the temperature of the reactants which enters, they are entering at T1 and it has been mentioned that the walls, the side walls of the reactor are perfectly insulated, so we are not going to have any heat loss or gain from the surrounding. So therefore the reactants, no reaction in zone 1, reaction endo or exothermic in zone 2 and again no reaction in zone 3. So we would assume that there would be some amount of heat generation or consumption of heat which has been denoted by Sc.

So SC is the whole matrix heat generation if it is an exothermic reaction that is taking place inside the reactor containing the catalyst particles. And our job is to find out T as a function of Z and other parameters and of course the other parameters would consist of the temperature of the at which the reactants are coming in, the amount of heat generation if it is an exothermic reaction due to the reaction and few other properties, few other conditions, such as what is a flow that of the reactants that is coming in and other factors.

But principally we would like to find out how does temperature varies axially in the reactor and whether having an exothermic in this part of would affect the temperature profile of the reactants entering the reaction zone or the temperature profile of the products leaving the reaction zone. So our basic aim in this issue of sin T as a function of the axial position in here.

Now if you look into this problem, you would realise that we are going to use, if we have to use a shell momentum balance, in the shell momentum balance, we are not going to have conduction, we also are going to have convective heat transfer, because there is a flow from left to right and this flow carries with it some amount of energy, so if I assume the control volume, somewhere in between, somewhere in the reaction zone, then some amount of energy will enter the control volume because of flow, some amount of energy will enter because of conduction, there would be a generation of heat inside the control volume due to the reaction and there would be 2 out terms, the convection out and the conduction out.

And if we consider steady-state conditions, then the sum, algebraic sum of all these terms must be equal to 0. So the 1st things, certain basic assumptions which one has to make in order to simplify the problem. We realise that this is a heterogeneous system, so any property that we refer to, is it going to be the property of the catalyst or the property of a gas mixture which flows past this catalyst particles. For example let us take the, let us take thermal conductivity.

So when we say thermal conductivity, which thermal conductivity are we talking about? Is it that of the gas, that of the catalyst particles or some sort of combinations of the catalyst particles and the gases which are flowing past the catalyst. So whenever we refer to any physical property in this, we are referring to some sort of an average property, for example the average value of thermal conductivity and so on. We also realise that this is a heterogeneous system, so somewhere you are going to have a solid particle, somewhere you have to have gas and so on.

So if you reduce the system size to differential element, then whatever we refer to in this specific problem would prefer to some sort of radially average property. So the other assumption, so all the property that we are going to use, we are going to refer in making the balance equation, the balance equation that means heat in minus heat out, plus generation is equal to 0 at steady-state, all the properties are radially averaged properties. Secondly, we will assume the temperature is not assumption of R, temperature is a function only of Z, that is the axial position but it is not a function of R.

And having the walls of the reactor perfectly insulated essentially helps, helps us in arriving or in using this condition, the temperature is not a function of R, it is only function of Z. So when we look back, look again at the diagram of reactor, what we then see is that temperature at any point is not a function of its location with respect to the side walls but of course temperature will vary axially as we move in as we move in the plus Z direction.

So if we are going to use a shell, then of course we have to use a shell whose, the smaller dimension would be the direction in which the temperature is changing. The temperature does not change with R, temperature changes only with Z. So the differential, so the shell across which we are going to make our heat balance, the conservation across which we are going to write the conservation equation will have a thickness, will have a thickness equal to delta Z, our it extends all the way up to R.

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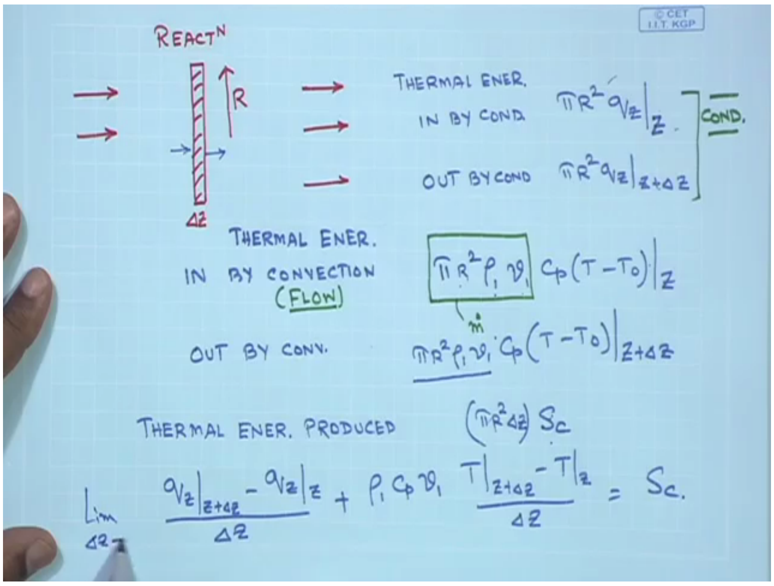

THERMAL ENER. IN BY COND $\pi R^2 q_z |_z$

OUT BY COND $\pi R^2 q_z |_{z+\Delta z}$ COND.

THERMAL ENER. IN BY CONVECTION (FLOW) $\boxed{\pi R^2 \rho_1 v_1} C_p (T - T_0) |_z$

$\dot{m}$

OUT BY CONV. $\underline{\pi R^2 \rho_1 v_1} C_p (T - T_0) |_{z+\Delta z}$

THERMAL ENER. PRODUCED $(\pi R^2 \Delta z) S_c$

$$\lim_{\Delta z \to} \frac{q_z|_{z+\Delta z} - q_z|_z}{\Delta z} + \rho_1 C_p v_1 \frac{T|_{z+\Delta z} - T|_z}{\Delta z} = S_c.$$

So think the, so if we take this and draw the shell of, it is a cylindrical shell of size delta Z in thickness and this is R, you have flow of reactants and products will go out and the reaction is taking place inside this shell. So if you consider this, then we have to 1st identify what are the mechanisms by which the heat can enter or leave. So when you think of a circular disk like shell which we have assumed through this side, I am going to have some amount of conduction, which, let us say we represent as Q suffix Z.

So that is a conductive heat flux which is entering the disk shaped control volume which we have assumed. So the amount of heat which comes in by conduction through the face of the disk, the left-hand side of the disk would simply be equal to the area time the heat flux, the conductive heat flux. So the area is simply pie R square and we are we denote the conductive heat flux by Q suffix Z and it is to be evaluated at a location Z.

So the amount of heat which comes in, the thermal energy, thermal energy which comes in by conduction would simply be equal to area pie R square times QZ which is the convective heat flux, it is evaluated at a location Z. And the thermal energy out, again by conduction, would simply be equal to the same thing, however QZ is now located, is now evaluated at Z plus delta Z. So these 2 therefore refer to the flow of heat into this shell due to conduction. So this is, these 2 terms are due to conduction.

And next we would see what is the thermal energy in by convection. And when we seek, when we mention convection, what I refer to is essentially due to the flow of the, flow of the stream, the reactants which are coming in to this shell. So the amount of material which comes into the shell must be equal to in volumetric terms the area multiplied by the local velocity. So area is pie R square and if I assume the local velocity to be V evaluated at Z, this will give me the total volume of reactant mass which is entering the, which is entering the disk shaped control volume due to flow.

So pie R square times velocity evaluated at Z is the amount, volume amount in meter cube per second which is entering the control volume. If I convert it in terms of mass, I simply multiply it with rho where rho is the density. So the mass flow rate of reactants and entering the control volume would simply be equal to rho times pie R square times VZ evaluated at Z. So that is the M dot. That is the mass flow rate which enters due to convection, due to flow. Now what is the amount of, what is the thermal energy which enters because of the because of the entry of this amount of mass into the control volume.

The simple expression is M CP delta T, where CP is the heat capacity and delta T is the temperature delta T is the temperature of the stream that enters the control volume minus a reference temperature, it could be any reference temperature but we have to be consistent in its use throughout our analysis. So energy is always expressed with respect to datum, so therefore the amount of convective heat that enters, amount of energy which is added to the control volume due to flow, due to convection would simply be equal to rho times pie R square times CP times temperature at location Z minus T0 where T0 is some reference temperature, some datum temperature which we are going to use for calculation of the energy content of the stream.

So the thermal energy in by convection due to flow as I said it would be pie R square rho velocity CP T minus T0 evaluated at Z. Now I could have used velocity at Z but what I what I have done is I have expressed rho at the entry conditions, velocity at the entry condition and this is the area. So this entire term that you see over here where rho and V refer to the conditions at this point, that is at the entry point where the density is taken to be equal to rho 1 and the velocity is taken to be equal to V1, so pie R square rho 1 V1 is essentially nothing but what is, what is the mass flow rate.

And since continuity has to hold in every, at every section of this reactor system, so whatever be the mass flow rate that is entering, it should remain constant so the the mass conservation will always be there as you move in this direction. So even if I reaction takes place, mass is always going to be conserved, moles may not be conserved because that would depend on the stoichiometry of the equation but mass will always be conserved at every section of the reactor that I have drawn.

So if I express my mass flow rate in terms of the entry conditions, the same mass flow rate will flow through every section of the of the reaction system. So therefore I express the mass flow rate in terms of pie R square rho 1 V1 where rho 1 and V1 refer to the condition at the inlet and as you can see this CP is the mass is the heat capacity, T is the temperature at location Z and T0 is some reference temperature.

So when we say, we evaluate out by convection, it would simply again be equal to pie R square rho 1 V1 as in the previous case CP T minus T0 but this is evaluated at Z plus delta Z. So this is the in term by convection, this is the out term by convection and these are the 2 terms which are expressed in terms of the entry conditions. And the thermal energy produced due to reaction, the thermal energy produced due to the reaction would simply be, since SC is the volumetric generation of heat, so this is heat generated per unit volume, so I multiply it with the volume of the of the control volume that we have chosen, volume of this disk which is pie R square times delta Z.

So this is volume, this is rate of heat generation per unit volume, so when you multiply rate of heat generation per unit volume with the volume of the system, what you would get is simply generation, the rate generation. And therefore if I take the algebraic sum of these, so in minus out, in minus out plus generation at steady-state would be equal to 0. And then as you can see pie R square will cancel from all the terms and you are going to divide both sides by delta Z, so what you have then is QZ at Z plus delta Z minus QZ evaluated at Z divided by delta Z plus this rho 1 CP V1 times T at Z plus delta Z minus T at Z divided by delta Z is going to be equal to SC.

So in minus out plus in minus out plus generation at steady-state would be equal to 0. Rearrange the terms, cancel the cancel these pie R square terms, divide both sides by delta Z and this is the equation which you going to get. So this is the difference equation that describes the flow of heat by conduction, the net flow of heat by conduction and the net flow of heat by convection and the heat generation term.

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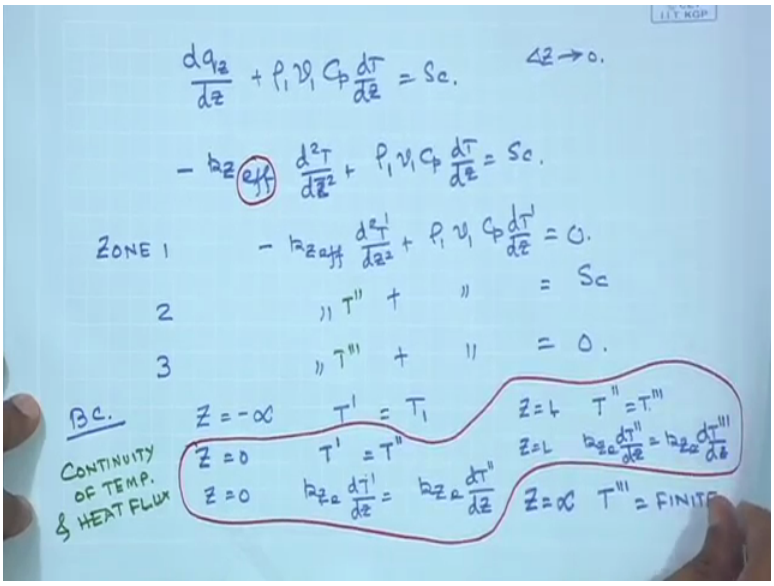

$$\frac{dq_z}{dz} + \rho_1 v_1 C_p \frac{dT}{dz} = S_c. \qquad \Delta z \to 0.$$

$$-k_{z\,\boxed{eff}} \frac{d^2T}{dz^2} + \rho_1 v_1 C_p \frac{dT}{dz} = S_c.$$

ZONE 1 $\quad -k_{z\,eff} \frac{d^2T'}{dz^2} + \rho_1 v_1 C_p \frac{dT'}{dz} = 0.$

2 $\quad$ " T'' + " $= S_c$

3 $\quad$ " T''' + " $= 0.$

B.C. $\quad z = -\infty \quad T' = T_1$

CONTINUITY OF TEMP. & HEAT FLUX

$z = 0 \quad T' = T''$

$z = 0 \quad k_{ze} \frac{dT'}{dz} = k_{ze} \frac{dT''}{dz}$

$z = L \quad T'' = T'''$

$z = L \quad k_{ze} \frac{dT''}{dz} = k_{ze} \frac{dT'''}{dz}$

$z = \infty \quad T''' =$ FINITE

So you take in the limit as L times Z tends to 0 and what you get out of this equation is simply the governing equation which is dQZ by dZ plus rho 1 C1 CP dT dZ is equal to SC. Now this is when delta Z tends to 0. Now we continue, we are we are assuming that it is a continue model, so continue is necessary to use this limit but we understand that the resulting equation describes average values of QZ, T, V, etc. So in order to use delta Z tends to 0, the system has to be uniform.

But we realise the system is not uniform, it has catalyst particles, then it has a wide space and so on, so we are imposing a continuum condition as delta Z tends to 0. That means the values that we refer to it this equation are essentially average values. This is something which we have to keep in mind. So we have this equation and then when you substitute QZ by Fourier's law, what you get is KZ but I would I would say this is the effective, put in the term effective because it contains, it takes into account both the, the solid particles as well as the work space times d 2T d dZ square plus rho 1, rho 1 V1 CP dT dZ is equal to SC.

So the equation will have different forming zone 1, in 2 and in 3. In zone 1, there would not be any heat generation term, so it would simply be minus KZ effective d 2T dZ square plus rho 1 V1 CP times dT dZ is equal to 0. In zone 2 these 2 terms would be there but this would be equal to SC, in those 3 the sum of these 2 would be equal to 0. And what are the boundary conditions that we use, we can use, that is at Z equal to minus infinity, that is when it enters the system T of zone 1, this is T of zone 1, T of zone, temperature of zone 1 would be equal to T1, this is entry temperature.

At Z equal 0, T of zone 1 must be equal to T of zone 2. And at Z equal to 0 KZ effective times dT1 by dZ must be equal to KZ effective dT2 by dZ. And the other one that you would get is at Z equal is L, that is at the junction Z equal L, Z equals L refers to the junction of zone 2 and so 3, the temperatures must be continuous, the heat fluxes must be continuous. At Z equals L, T of 2 must be equal to T of 3 and at Z equal to L, KZ effective d T2 by dZ must be equal to KZe dT 3 by dZ.

So this is the 3rd condition and at the other end at Z equal to plus infinity, T3 must be equal to finite. So the 6 boundary conditions, these refer to the conditions, the temperatures are same, the heat fluxes are same at the junction between 1 and at the junction between 2 and 3, IZ equals L, temperatures are same, the heat fluxes are same. So these are essentially continuity of temperature and heat flux. So the 3 equations, the 3 equations referring to temperature at 2, and temperature at 3 and temperature at 1, the terms would be, the other terms would be the same, these 3 questions would have to be solved with these 6 boundary conditions.

You can see the solution of this linear textbook of Bird, Stuart and Lightfoot, this problem has been solved in Bird, Stuart and Lightfoot, so you can take a look at that. The solution methodology from this point essentially involves the converting these equations in dimensionless form, converting the boundary conditions in dimensionless form and use simple logic to obtain what could be the temperature profile. It is not difficult but you simply have to see the different steps, I will read talk about the fundamental steps when you require some understanding.

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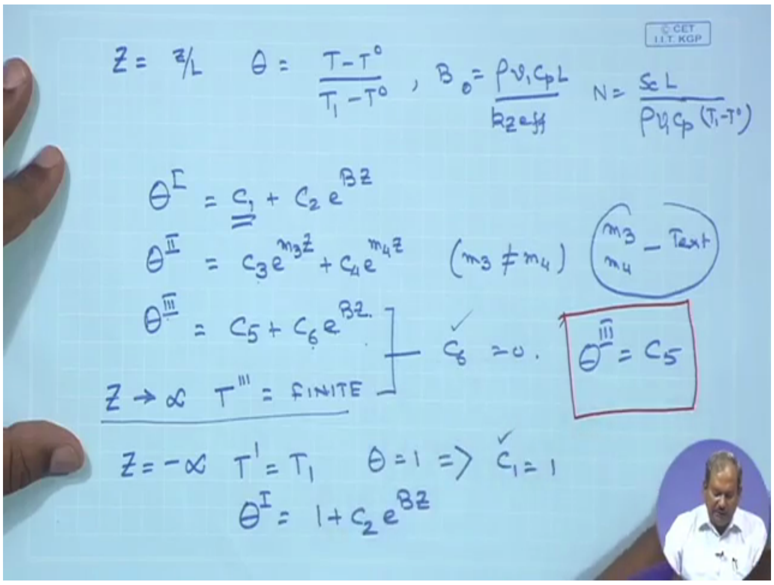

$Z = z/L \quad \Theta = \frac{T - T^0}{T_1 - T^0}, \quad B_0 = \frac{\rho v_1 C_p L}{k_{z\,eff}} \quad N = \frac{S_c L}{\rho v_1 C_p (T_1 - T^0)}$

$\Theta^{I} = \underline{\underline{C_1}} + C_2 e^{BZ}$

$\Theta^{II} = C_3 e^{m_3 Z} + C_4 e^{m_4 Z} \quad (m_3 \neq m_4)$ m_3, m_4 – Text

$\Theta^{III} = C_5 + C_6 e^{BZ}$

$Z \to \infty \quad T^{III} =$ FINITE

$C_6 = 0. \quad \boxed{\Theta^{III} = C_5}$

$Z = -\infty \quad T^{I} = T_1 \quad \Theta = 1 \Rightarrow C_1 = 1$

$\Theta^{I} = 1 + C_2 e^{BZ}$

So the equation is a nondimensionalized and the boundary conditions are nondimensionalized and are used as I am going to show now. So what is done is that the, new dimensionless numbers are Z by L, Theta the temperature is T minus T0 where T0 is the reference temperature and there are other terms be which is rho V1 CP L by KZ effective and N which is SC L by rho V1 CP T1 minus T0. These equations, the 3 equations were then solved to obtain Theta 1 is equal to C 1 Plus C2 e to the power BZ.

The temperature profile for zone 2 would be equal to C3 e to the power M3 Z plus C 4 e to the power M4 Z, M 3 is not equal to M4 and Theta 3, the dimensionless quantity temperature in zone 3 would be C5 plus C6 e to the power BZ. Now the different values that you can, the values of M3, M4, etc. are given in your texts, so I am not writing them over here. Now as Z tends to infinity, we understand that T3 is finite, that is the boundary condition which we have identified over here, that at Z equals infinity, it really at the exit of the reacting systems, T3 has to be finite.

So if we see here at Z equals infinity, T3 has to be finite, so and if you see this equation, these 2 clearly tells you that C6 would be equal to 0. So in order for the temperature to be finite, that means dimensionless temperature of reacting mixtures in zone 3 to be finite, the C6 has to be equal to 0, so which gives you Theta 3 is equal to a constant. So this is the 1st observation even without solving it which you can write. And the other one that you can you can do is the at Z equals minus infinity, T of 1 is equal to T 1.

The temperature of zone 1 is equal to the temperature at which the reactants enter the reacting system, the reaction system which would simply tells you the Theta is equal to 1 and this would give rise to C1 which is this one is equal to 1. So the 3, the Theta 1 is simply going to be one plus C2 e to the power BZ. So C6 I can clearly find out, easily find out from the understanding, C1 can be found out and using the other boundary condition, C3, C4, etc. can also be found out.

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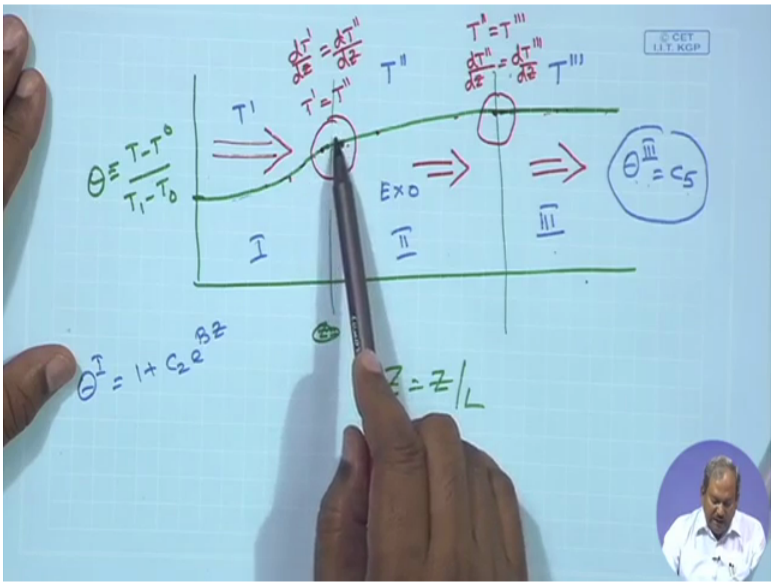

The plot of this temperature profile which is Theta defined as T minus T0 by T1 minus T0, when, so this is Z equals Z equals Z by L and these are the 3 zones. So what I have seen here is that Theta 1 is equal to1 plus C2 e to the power BZ and C6 equals to 0, which gives me the temperature in the zone 3 will remain a constant. So temperature in the zone 3 will be a constant. Temperature in zone 1 is slowly going to rise till it enters zone 3 where it is going to increase, since it is an exothermic reaction and will asymptotically merge with 3.

So this is T3, this refers to T2, this refers to T1. So there is no problem in understanding T2, since there is an, this is an exothermic reaction, so the temperature of the reactants and products mixture will increase. Our analysis tells me that Theta 3 is equal to C5 which is a constant, so the temperature of this zone, so 3, this is zone 2 and this is so 1. So temperature of zone 3 will not change, it is a constant. However if we look at the temperature of zone 1, which has been given by 1+ C2 e to the power BZ, the temperature of zone 1 will slowly increase.

The conditions that are to be maintained at these 2 junctions are that T1 at this junction must be equal to T2 at this junction. The dT dZ at this point must be equal to dT 2 by dZ and similarly at this you have the temperature equality and the these 2 would be equal. So the last condition gives me it is a constant profile, if it is a constant profile it has a 0 slow, so from on this side it should approach the junction between 2 and 3 with a 0 slope. Okay. So this condition is to be maintained.

Whereas the condition over here is like this, temperature equality and gradient inequality. So since no reaction is taking place in so 1, how come the temperature is increasing? That is the only question that we need to answer. You have flow of gas, the reactants in this direction. The reactants and products in this direction and the products are going out in this direction. However the temperature at this point is more than the temperature at this point.

So the convective flow is going from left to right at due to this temperature difference, there will always be a conductive heat transfer which will which will be in the direction from 2 to 1. We have to, if you understand that, then this part is, this part is, this is this is very clear. The convection is from left to right but due to the difference in temperature, since it is an exothermic reaction is taking place over here, so the temperature at this point must be greater than the temperature at this point and whenever there is a temperature difference, there would be a conductive flow of heat which you cannot stop.

So the entering reactants are going to be preheated due to the exothermic nature of the reactions which starts at zone 2. So zone 2, the entry of zone 2 will result in an increase in temperature of the mixture. Since the temperature is more, the one the this stream which is entering, even though no reaction is taking place, this is going to receive some amount of energy from the higher temperature mixture of reactants and products by conduction.

So convection is in this direction but at the junction between 1 and 2, we may have conduction in the reverse direction, reverse to that of flow, reverse to that of convective heat transfer, which would result in the preheating of the mixture which is entering the reaction zone, that is reaction 2. But when we consider the junction between 2 and 3, we do not have any such condition because in the zone 3, the temperature is constant and the zone 2 temperature approaches the junction between 2 and 3 with a 0 slope.

So we do not have it difference in temperature between the 2 side of the junction 2 and 3 and the 3 side of junction at 2 and 3. So therefore we do not have any conductive heat transfer in between zone 2 and zone 3 at the boundary between the 2. So there is no question of change in temperature beyond zone 2 when we enter zone 3. So there may be preheating if it is an exothermic reaction, a cooling effect if it is an endothermic reaction but since it approaches the junction of 2 and 3 with a 0 slope, there is not going to be any change in temperature or any effects of zone 2 on zone 3 except for a constant temperature which is going to be higher for exothermic and lower for the endothermic reaction.

So this example essentially gives you an idea of how to use the shell when both conduction and convection are present, the concept of preheating or precooling when we have some amount of heat generation or consumption, exothermic or endothermic reaction in a reactor. So in the next class we will pick up another problem, another interesting problem like this.