Mathematical Modelling and Simulation of Chemical Engineering Process
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Lecture 02
Introduction Continued

Hello and welcome to the second lecture on this course of Mathematical Modeling and Simulation of Chemical Engineering Processes. We will continue from where we left in the last class, and we will try to show you another example from heat transfer.

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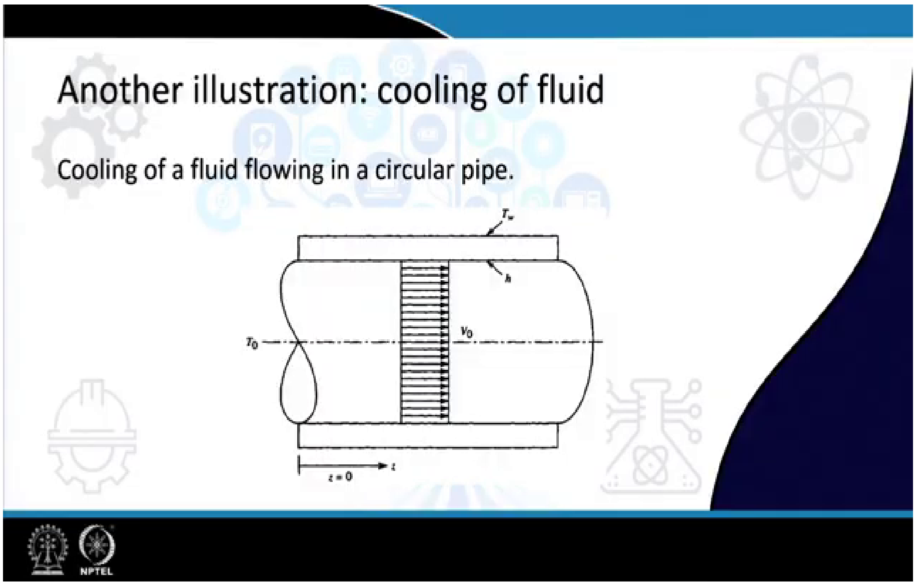

So, all of you are aware of a fluid flow in a pipe and this is a very relevant problem particularly in the context of heat exchangers, whether it is double pipe or shell and tube exchangers, that heat transfer of a flowing fluid in a pipe. So, let us assume let us consider that you have this pipe where there is a flow of the liquid in this pipe and we are trying to model the temperature in this pipe and the idea of the objective is to find out like how the temperature decreases with the actual length of the pipe. So, let us try to make a try to frame the model and as you know the first step in framing the model is the assumptions.

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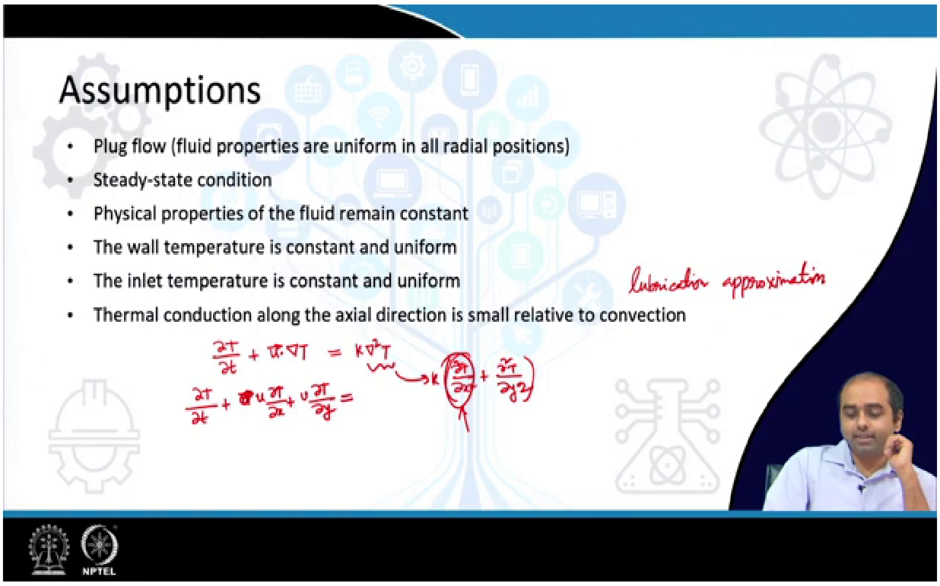

So, here is the list of assumptions that I have thought of at this moment. And I have included several assumptions to simplify the problem. Many of these assumptions as you can see, for example, the steady state condition or the criteria of the plug flow of the fluid is actually to simplify the problem rather than you know try to relate the actual scenario, of course, in the actual scenario, it is not a steady state problem, it is a dynamic problem.

Flow is not plug flow you have, this parabolic flow profile, but for the first stage or the at the first attempt, let us try to simplify the problem and then slowly let us try to relax the assumptions. So, the condition of steady state simply implies that there is no time dependence in the problem. We also assume that the flow properties of the fluid are constant.

So, all these density, viscosity, thermal conductivity, etc., do not change with temperature, this is often not the case when you have gaseous system particularly the wall temperature is maintained to be constant. So, it is a constant wall temperature problem and there is another option to have a constant heat flux. The inlet temperature inlet temperature of the fluid is also constant it does not change with the time or any process fluctuations.

The last point is very important we consider that the conduction along the axial direction is small or is negligible compared to the compared to the convection. Now, this is to some extent is related to what we know by the lubrication approximation and you know this that and how and what do we essentially mean in terms you know, the mathematical idea is that if

I try to write the heat transfer equation. So, this u is the velocity vector. Maybe I should write vector with some some arrow mark here at the top is equal to k grad square T.

So, this k grad grad square T part, if it is expanded in the Cartesian or in terms of the radial coordinates what you will see that this is what we generally get in terms of the Cartesian coordinate K into and the left hand side is for a 2 dimensional system I am talking about it is u dT dx plus V dT dy.

So, what I am suggesting here is that along the axial direction, let us say x is the axial direction to the problem. In this axial direction the conduction the heat transfer due to the convert conduction is very small compared to the convection and this can be proved, for long cylinder pipes that if the aspect ratio of the pipe is very small, generally the axial direction conduction or the double derivative terms in the axial direction is very small because it is in the order of the aspect ratio square. And this can be ignored with respect to the other terms. So, this is even though an assumption it is quite practically relevant.

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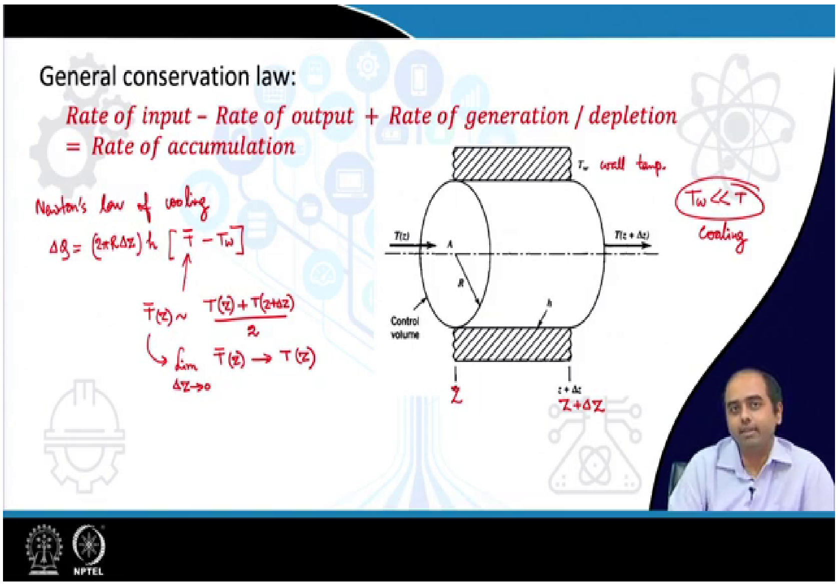

Now, moving ahead to the model, this is kind of the mental picture that we have in mind. A small section of the tube across which the heat transfer takes place that this is at a location of Z. So, we are considering the axial direction as Z, do not get confused with x. So, this is at a particular location of Z and the small elemental section is Z plus Delta Z. So, the temperature of the fluid entering this part of this small section is T(z) and whatever is leaving is T(Z plus delta Z), the wall temperature is denoted as T w and this is held constant.

So, here simply try to make, you know energy conservation. So, the energy conservation tells you or any any conservation law tells you that the rate of input minus the rate of output plus the rate of accumulation as our rate of generation is equal to the rate of accumulation. So, here we try to apply the same thing there is no rate of there is no heat generation there is no heat accumulation. So, it is only the rate of heat loss and is equal to the rate of heat input. So, how do we like the rate of heat loss, it is from the Newton's law of cooling.

So, you all know that it is dependent on the heat transfer coefficient h. So, we write the 2 Pi r Delta Z. So, this is the cross sectional sorry the circumferential surface area of this elemental section, Delta Z multiply with h and the difference of T minus this Tw. Of course, I should write here that this is the case of the cooling, so, Tw is less than T for the problem.

So, the in writing the rate of ease plus since T is higher we write T minus Tw and what is this T bar? So, T bar is the average fluid temperature in this cross section and how do we write this. So, this T bar (Z) is the average of the inlet and the outlet, by 2. So, if I try to write limit Delta Z tending to 0, this T(Z)bar is equivalent to T of Z. So, this is the part after heat loss now, this will be equated to the in minus out of the enthalpy.

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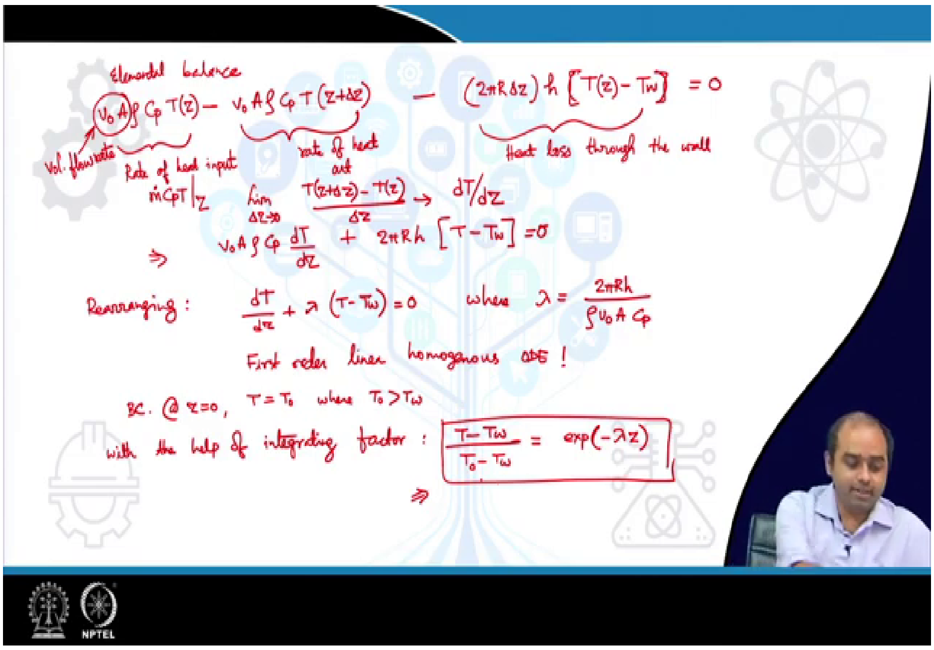

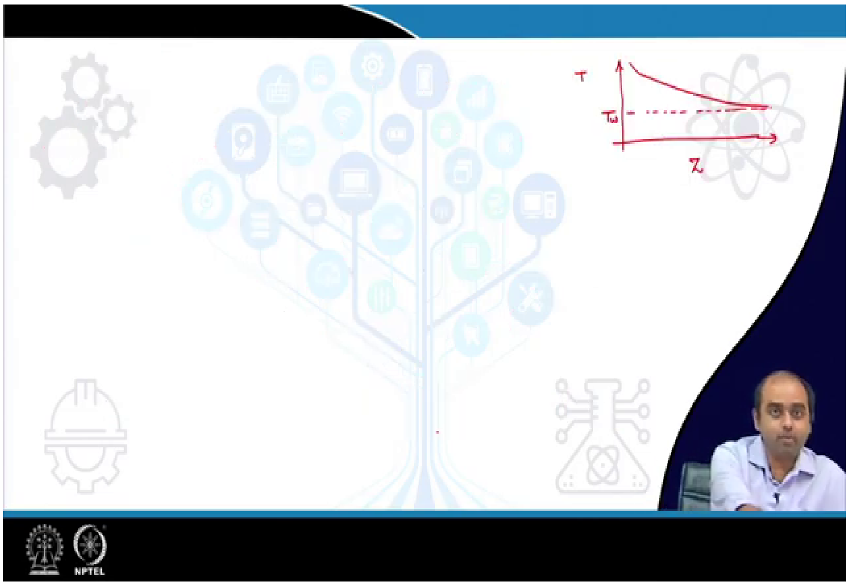

So, this is the amount of the heat loss. Next we try to write our elemental heat balance for this case. So, this is the say the volumetric flow rate is V0 A, A is the cross-sectional area in this case rho Cp. So, V0 A, into rho this tells you what is the V into A is nothing but volumetric flow rate. So, V0 is the linear velocity multiplying with the cross-sectional area will give you the volumetric flow rate you can also write it in terms of volumetric flow rho Cp T at Z minus V0 A rho Cp T at Z plus dZ.

So, this is the rate of heat input into this section of Delta Z and you can also write is m dot C p T is at Z and this is the part of rate of heat out, heat or enthalpy out you can say, minus the heat loss. What is this heat loss we have already done 2 pi R from the Newton's law of cooling h and this T, I will write it as Tz minus Tw. So, it is the rate of heat loss. So, this is the part of heat loss through the wall.

So, if I you already know the next steps. I just try to reorganize this and I can write V0 A rho Cp dT dZ. So, you if you assume that you know in the limit of delta Z tending to 0, this T of Z plus Delta Z minus T(Z) divided by Delta Z, is nothing but the total derivative of temperature with respect to the axial coordinate, plus 2 Pi R h T minus Tw equal to 0.

So, just rearranging little bit. So, on rearranging the above equation I can write dT by dZ plus lambda into T minus Tw is equal to 0, where lambda is equal to 2 Pi R h by rho V0 A Cp. So, now this is a first order, so, first order linear homogeneous ODE and you can easily solve this equation with the help of the integrating factor.

So, let us define the boundary conditions for this problem since the first order in z, so only one boundary condition is sufficient at z is equal to 0. At the inlet of the pipe let us say that the T is equal to T0, where of course T0 is greater than Tw, that is why the cooling will take place. Now, with the help of the integrating factor, you can just solve this equation and this is something which you have already studied in your high school.

So, I can straight away write the solution to this equation as a slightly different way I am writing. This is solved using the help of the integrating factor and you can see that the temperature in this problem decays with this Z. So, if I will try to plot the temperature profile with respect to the axial coordinate. So, if I try to plot the temperature profile and it will be coming something like this. So, this is Tw.

So, some of the important conclusions that you can interpret from this equation is that not only does this equation tells you that, how does the temperature you know vary with the axial position you can also have an inverse idea, like what should be the length of the pipe so, that I can drop the temperature to this value of the inlet condition.

Let us say you want to decrease the temperature by 10 degrees, you will let us say the inlet temperature is 100 degrees of the say 100 degrees of that liquid that is flowing and the wall temperature is maintained as 30 degree, and you want to reduce it from 100 to 50 degrees.

So, in that case what is the minimum length required in that tube so, that is what we call it the inverse problem they are trying to relate that at what length you will be getting what temperature so, that that can help you in the design also of this length of the tube required to have a certain drop in the temperature. So, apart from knowing the temperature profile with the actual position, you can also calculate the inverse problem and find out that what is the minimum length required for a particular drop in the temperature.

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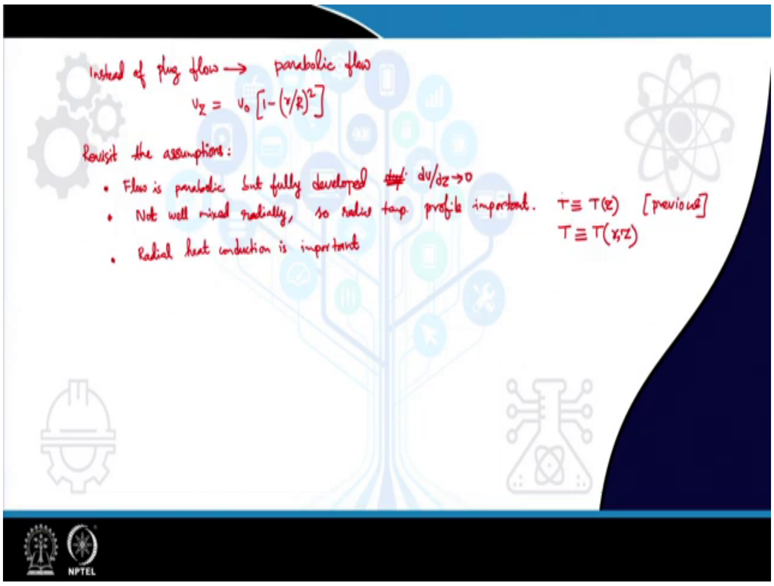

So, now moving ahead now moving ahead in the case that instead of the plug flow. So, instead of plug flow, let us say, we have parabolic flow. Because the condition of plug flow is not true always. So, in most cases you are expected to have a parabolic flow and you know that if you have a parabolic flow the velocity profile would be looking something like this, 1 minus 1 by R square.

So, if I try to revisit the assumptions, what are the things that I will see, is that the fluid flow profile is not a parabola is not plugged flow it is a parabolic profile, it is not so the flow is parabolic in nature, parabolic path fully developed. I hope all of you realize what do you mean by fully developed we say that this dU sorry dV by dZ is equal to 0, that is what I mean by fully developed, it does not change with the axial direction.

Next is we are saying that it is not since there is you know radial component of the velocity or the velocity is not same at different radial location. So, it is quite obvious that it is not well mixed radially. So, the radial temperature, so radial temperature profile is important. So, this is now our change. So, in the previous case T was actually a function of Z. This is the previous scenario we have just completed and in this case T is not only a function of Z it is also a function of R.

So, this is the important consequence and next thing that we say is that in this problem whatever the axial heat conduction that we have said may not be true, because since there is a profile in the radial direction, radial heat conduction may be important. So, we cannot completely disregard conduction in this problem, we can have radiant heat conduction to be conduction to be important.

So, this was important. In the previous case the entire conduction was actually scrapped out from the equation because we felt that you know conduction is negligible compared to convection in the problem and you know that these criteria can be enforced when the piclet number is actually very large. But now, it is it may not be the case only the radial heat conduction may be important, but still with the help of lubrication approximation, you can say that the actual heat conduction may still be negligible. So, only the radial heat conduction is important. So, now, in this problem, we once again try to you know write down the shell balance to this equation.

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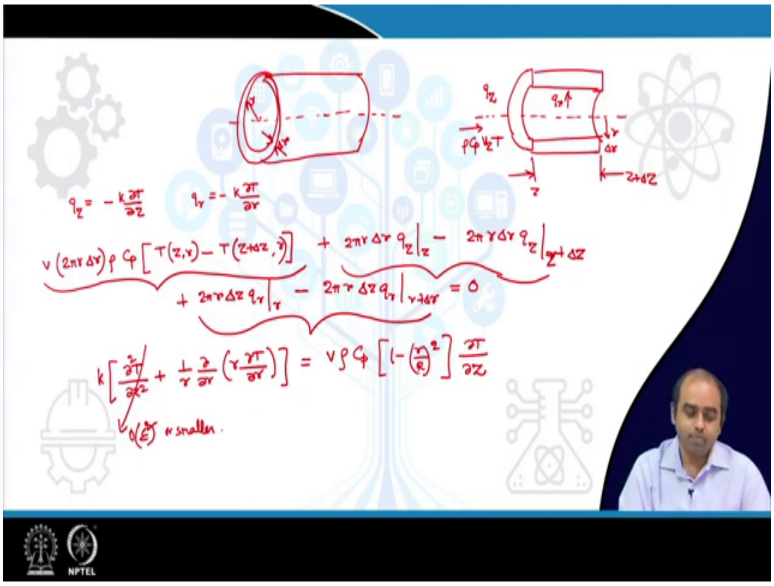

So, what we see is that you try to make a shell balance. So, let us say this is as small I could not draw it properly, but I hope all of you get the entire essence. So, we will have a small cross section of r sorry of section delta r and also there will be a section of delta Z. So, both I am trying to draw together and to give you a perspective, that is not only r but also in the Z direction. So, it will look something like this. So, this is like Z and you are having this as Z plus delta Z and this is r and this is delta r.

So, you are having qz coming in and you are also having qr in the radial direction and this is the enthalpy due to the inlet velocity. Now, q is from Fourrier law of heat conduction you can write qz to be minus k dT dz, qr to be minus k dT dr. So, if I try to make a cell balance across the r as well as across the z direction what I get is that V 2 Pi r del r rho. So, this I am trying to write in the r direction sorry, this is the inlet part I am trying to write first. The Z direction, next time trying to write the conduction part also. And then later on we can say which conduction to be kept and which one can be ignored, qz at z minus 2 Pi r del r, qz r plus sorry z plus del z plus 2 Pi r delta Z qr. So, this is the r direction conduction. 2 Pi r del z q r r plus delta r, sorry r plus delta r, is equal to 0.

So, of all of you can realize the first part, the first part is the rate of, so, this part is the convection part. This is please note that now, temperature is not only a function of z but also a function of r. So, the first part is you know enthalpy into the problem and then in the next part of the problem, the next terms denote to the conductive, so, these parts are the conductive heat in and conductive heat out in the axial direction this is the conductive heat in and out in the radial direction. Now, please note that here we do not include or do not bringing the Newton's law of cooling in this problem because that will come as a boundary condition in the r direction. So, this r direction is not exactly at the boundary, but somewhat inside the problem.

So, that condition of the surface what is happening or last through the surface is not coming in the picture. So, the entire here there is enthalpy or the fluid enthalpy due to the convection between the inlet and outlet z and z del z plus delta z is balanced by the conductive heat transfer both in the z and the r direction.

So, if you take out all the if you do all the limits of delta tends to 0, delta z tends to 0, you can simply find out that you will be getting the equation the conductive this heat transfer equation something like this. By lubrication approximation, this would be order of epsilon or smaller order of epsilon square in fact. We can ignore this term and we can say that the actual direction heat conduction is not important, but radial direction heat conduction is important.

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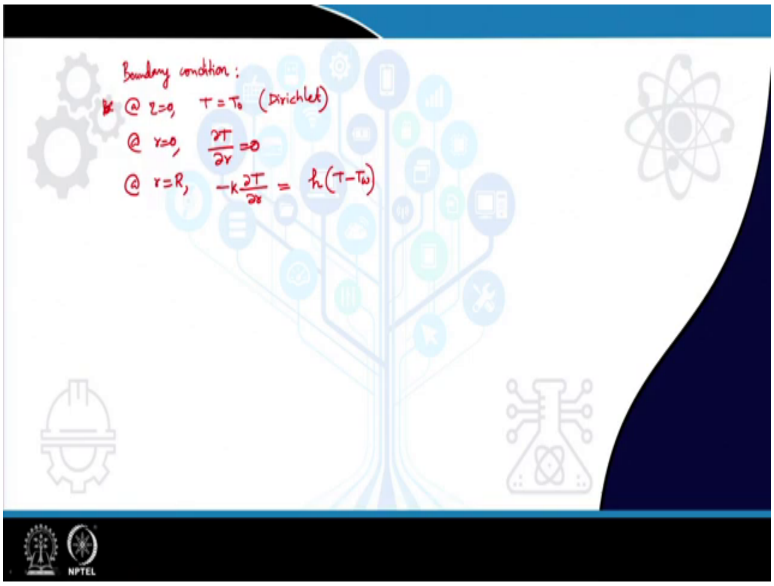

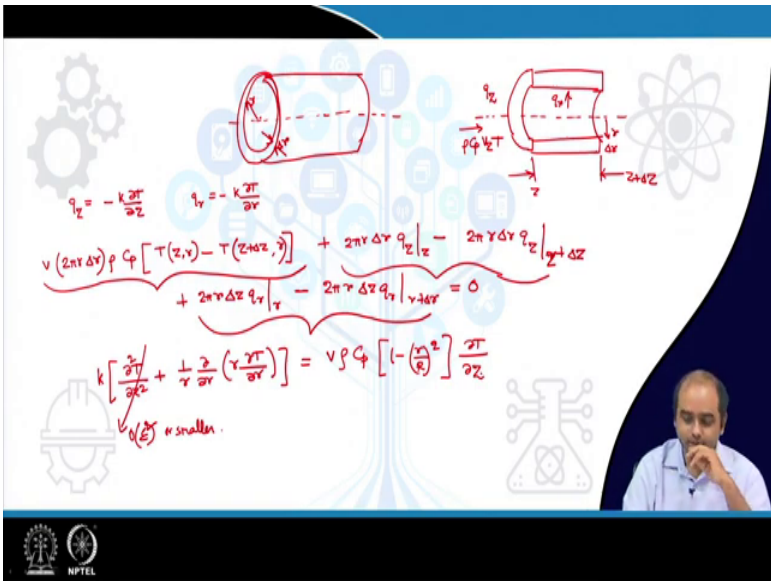

Now, we are trying to write down the boundary conditions. So, please note that this problem is second order in r and it is essentially a PDE now. So, you will be having 2 boundary conditions in R and 1 boundary condition in Z. So, at Z is equal to 0, you will say that T is equal to T0 and this is the all of you are aware of this that this is the dirichlet condition at r is equal to 0, you will have the symmetry condition which is dT dr is equal to 0 and at r is equal to the surface you will be having the mixed boundary condition and this is where the Newton's law of cooling will be coming into the picture.

So, all the fluid properties are constant. So, the conductive heat transfer is balanced by the, you know the convection at the surface. So, this is how you are going to frame the problem. So, of course, this is a partial differential equation which cannot be solved just at the blink of an eye or straight forward and we will talk about in the upcoming lectures on the review of the partial differential equations and how we can solve such linear PDE with analytical techniques as well as new numerical techniques for nonlinear PDEs.

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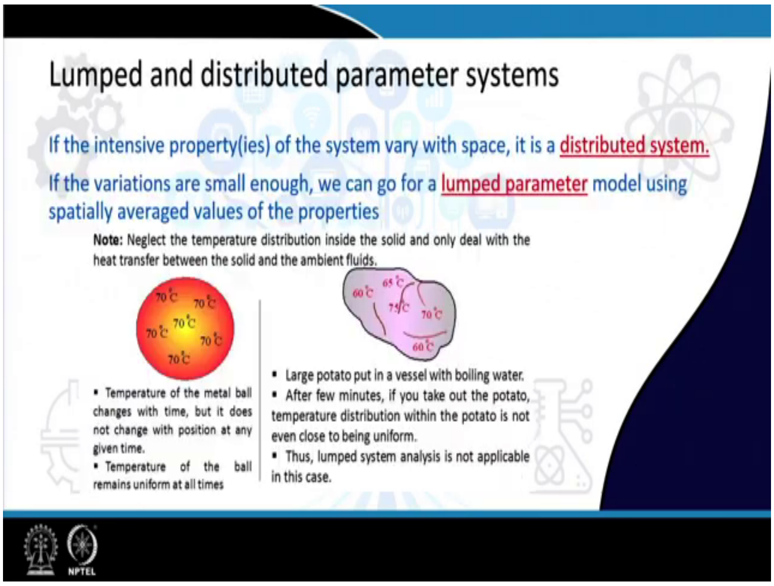

So, with this I would like to move ahead further and talk about the lumped and the distributed parameter system. So, far we have seen this cooling of the pipe, cooling there we have seen that it is mostly a distributed parameter system or if you can also consider in a slightly different way the first problem where you know it was only varying with respect to Z, you can consider it is lumped in one actual direction but anyway, let us not confuse ourselves.

We say that our distributed parameter system is important when the system properties or the characteristics vary with space and not only with time. In the lumped parameter system, it only changes with the time. A classical example is that if you have a ball having high thermal conductivity, it is expected that the temperature distribution inside the solid would be much much faster or there is you know sorry not faster if we mean the temperature would be uniform inside the body and it does not change with any given position.

So, that is what we call as a lump parameter system. But if you have a very small thermal conductivity, it is expected that the inside is not uniform fast. It will take considerable amount of time before the temperature inside is uniform and in this case the lumped analysis model is not applicable.

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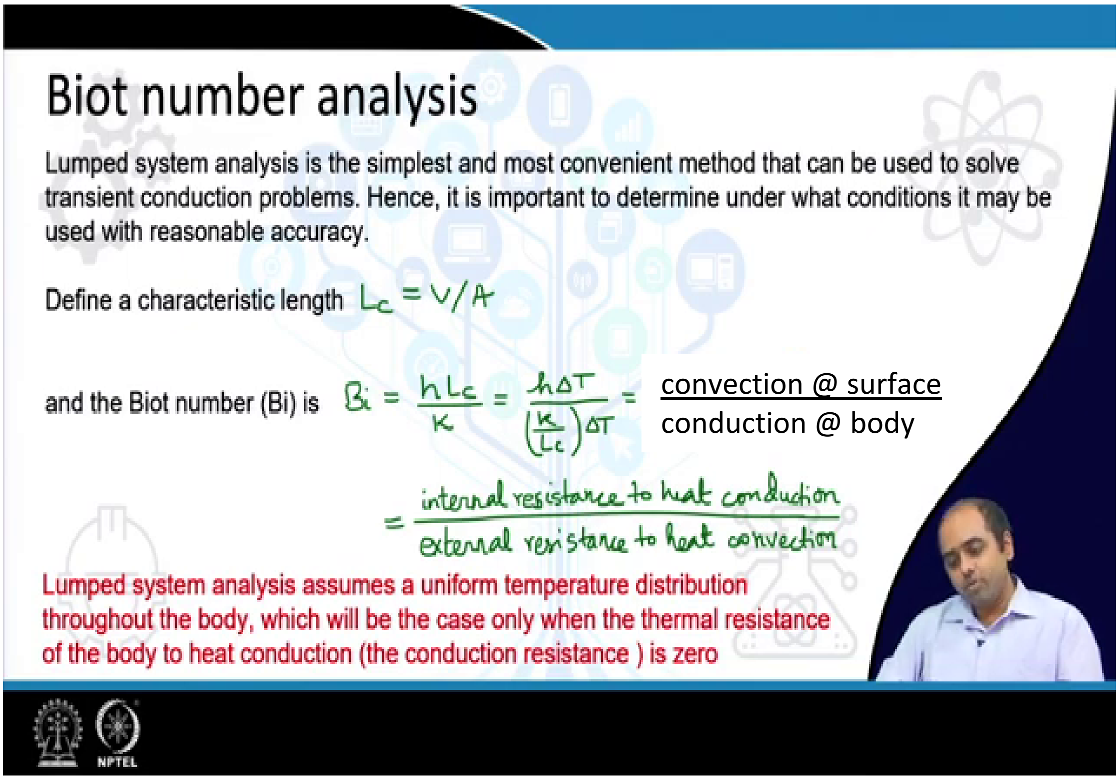

So, the important criteria to distinguish whether a problem is lumped or distributed is to use the Biot number and most in most cases this is used in the context of heat transfer only. So, the Biot number essentially is the ratio of the internal resistance or the internal resistance to heat conduction with respect to the external resistance to heat convection and this can also be represented at the convection at the surface vis-a-vis to the conduction at the body.

So, if the Biot number to the problem is very very small, if the Biot number to the problem is very small, then essentially it is a lumped parameter system. And if the Biot number is large and how small or how large is again a matter of you know, it is a relative matter generally for Biot number less than 0.1 or 0.05, we can consider it to be a lumped parameter system. So, this is the category of the distributed and the lumped parameter system.

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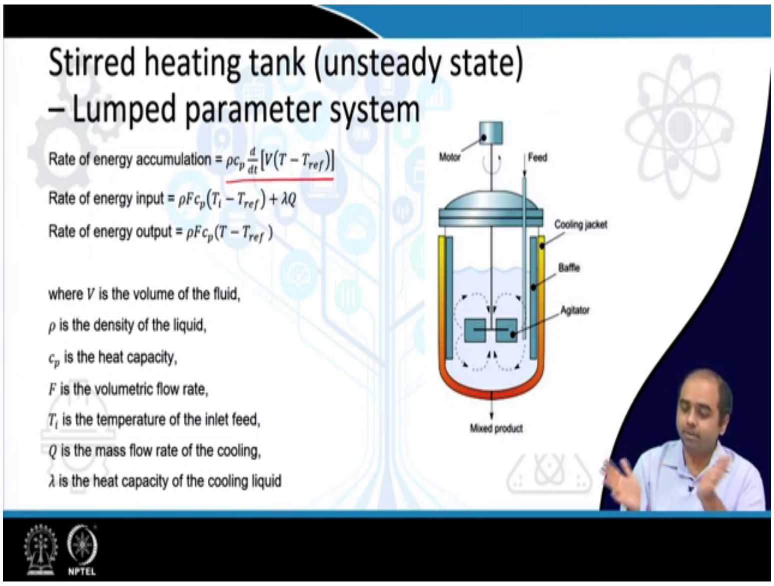

And as you can see, we will also have one small example on the lamp parameter model. So, far we have been discussing mostly the distributed parameter system. So, this is a heating of a stirred tank system and we consider that it is well mixed. So, the temperature distribution in this tank is not important only we want to find out the dynamics of the temperature how the temperature evolves.

So, you can see that the rate of energy accumulation is equated to the energy in minus energy out. So, and if there is any rate of energy generation to the problem, so, there is no spatial variation or we do not write temperature as a function of the spatial coordinates in this problem. So, this is an example of a lumped parameter or unsteady state I mean essentially a time dependent system where we have the rate of energy, sorry, the change in energy only with respect to the time and the temperature field is not changing with respect to the space.

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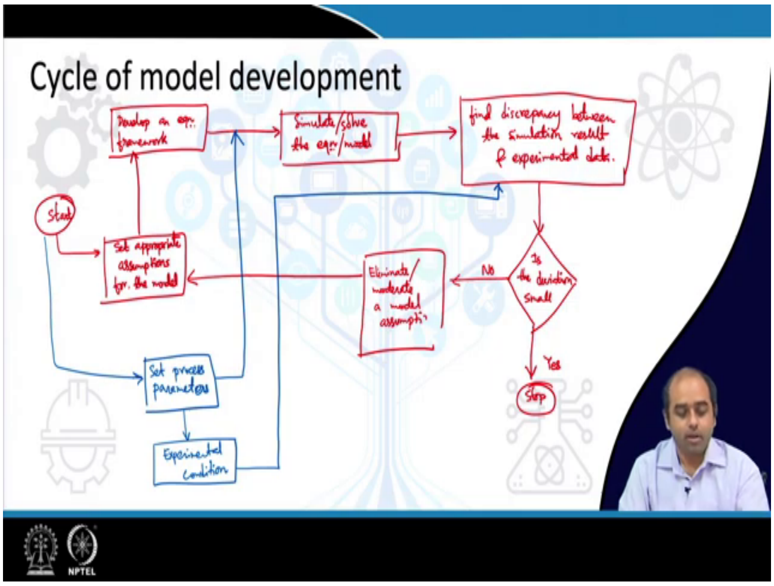

Now, coming next I want to talk about a little bit on the cycle of model development and how do you actually frame a model. So, the first starting point, let me try to draw you know process or the algorithm scheme. So, from the start, you set appropriate assumptions for the model. So, this is the first thing that you need to do for the model approach or the modeling approach.

Next thing that you do is that develop an equation framework and of course, the next step is to simulate or solve the equations are the model equations and the next step is to find discrepancy between the simulation result and any experimental data. This is very important simulation result and experimental data.

So, this is what we call as the validation of the model. So, these discrepancies are the deviations of the model results could be due to many things it could be due to the assumptions that has been considered, it could be due to the inaccurate value of the properties, it could be your solution algorithm also, but whatever you try to find out that deviation or the discrepancy.

So, next thing is to check that is the deviation small, this is a check. So, if this is yes then you stop. Then you say that your model is quite well nicely prepared and it can you know nicely predict the experimental observations. But if it is no then generally you eliminate or moderate a model assumption and then again you set the appropriate model equations and then you continue.

So, there is also one more part to the problem which I must highlight here and possibly in a different color let me try that you would also need to set up the process parameters. So, apart from the assumptions you have to also set the process parameters and this would be used here and this would also be needed for the experiment.

So, with this same process parameter or whatever the experimental process parameter is there, using the same process parameters, you have to also set the process parameters accordingly. So, what I mean is that the process parameters in the experiment as well as in the model simulation should be same.

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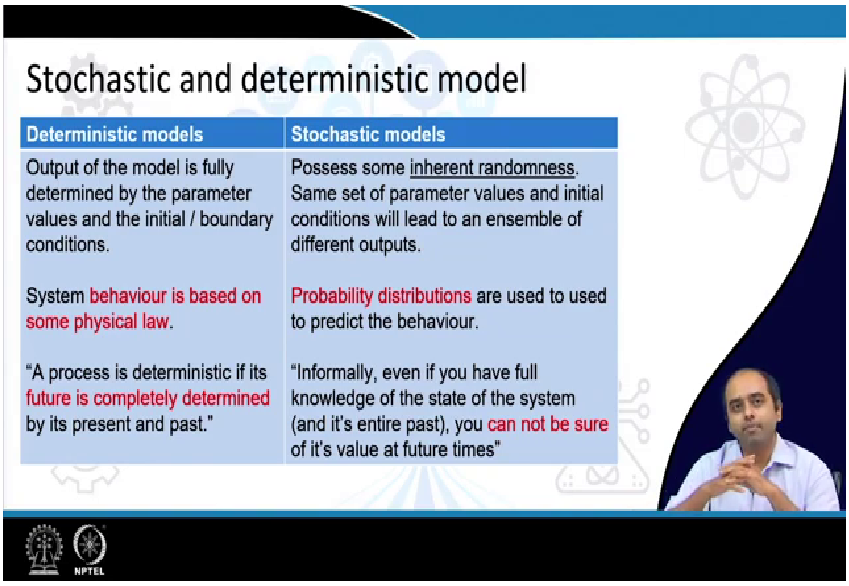

Finally, I want to talk about the last classification of the model which is the the type of what we known as the stochastic and the deterministic model. So, far we have been talking about most of these models as deterministic and the deterministic models are actually described by a physical law very nicely it is described by a physical law and the process or the future of the process is completely determined or known by its present and the past. In the case of stochastic model, there is some randomness in the system due to which you cannot (you know) with absolute certainty you cannot predict the future.

So, there will be always some probability distributions or some probability factors assigned to the results. And it is not entirely that whatever the result that you get out of a stochastic model is wrong are correct, but there is a degree of correctness to the final answer and you cannot be absolutely sure of the value at future times.

So, stochastic models are only preferred or only should be preferred when the system cannot be described by a physical law or clearly by some known physical (you know) model or based on some physical law or the system is too complex that there are so, many you know coupled phenomena is happening that is almost theoretically at this point of time impossible to frame explicitly the mathematical equations. So, this is the case, or this is the condition under which one should prefer approach for the stochastic model sorry stochastic model.

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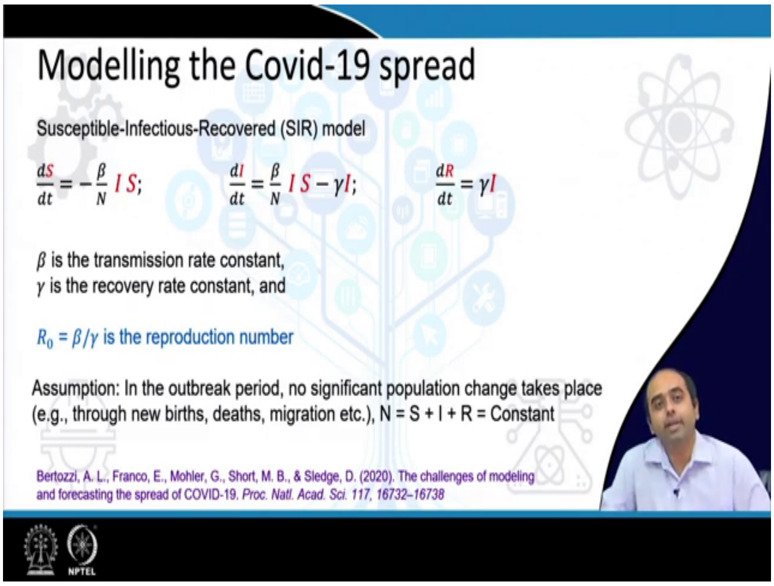

Now, this stochastic model I mean that one of the brightest or the, I would say nice example in present day times can be in order to model the COVID-19 spread. So, this pandemic spread or the infection trend is something which is very random in nature it cannot be dscribed by any physical law. And there are so many factors which affect this spread or the spreading dynamics of the model. And to model such systems you need to take into account of some you know, stochastic type of model. So, stochastic models are essentially also some mathematical equations. But these mathematical equations are not related to any physics but I can approximate the trend behavior of the model.

So, this is one very popular COVID-19 model which is known as a susceptible infectious and recovered model. So, a fraction of the population is considered to be vulnerable to the virus, a part will be infectious and only a part of this will be recovered. Of course, there are a lot of assumptions in this model, we do not consider the death rate as a separate parameter.

So, well so, recovered could also be the you know persons who are passed away. Similarly, the entire population is essentially considered can be considered to be susceptible or can be a fraction of the entire population to be considered as susceptible and also a total population in the outbreak should not change with time that we in the period in which we are modeling the virus dynamics.

So, the susceptible infection and the recovered, these all 3 of them the addition of all 3 should be constantly essentially means that there should not be any new birth are any migration or any change in the population or if there are any deaths in the population they can be I mean recovered can be same as deaths also. So, this is the SIR model. And in this model, you see that there are some constants one is beta 1 is gamma. So, beta is typically determined as the transmission rate constant and gamma is the recovery rate constant.

So, gamma is inverse of the time and beta is the transmission rate constant and the ratio of these two the beta versus gamma is typically known as the reproduction number. So, if the reproduction number is greater than 1, it is mathematically established, that the outbreak is going to be and that there is outbreak and the pandemic and the virus transmission is likely to grow.

So, if the transmission rate exceeds the recovery rate, that is what this ratio tells you reproduction number, it is difficult to contain the virus and that is what we mean by the reproduction number. You can easily try this model yourself. This is the set of three ordinary differential coupled ordinary differential equations and from the different you know waves - first wave, second wave third wave you can you know try to fit this model equation and get the different reproduction number values and that will tell you that how does this the recovery rates are. How does this model or how it can help you to predict the trend of the infection. But please note this is a stochastic type model.

There are also several different types of stochastic models available based on based on random number generators. For example, this is what we call a random Markov chain model. There are some several other random models which are also can be used to for this COVID-19 model spread. Anybody interested can go through the reference mentioned below and you can look into more details of this SIR model.

So, with this, with this I conclude on the introductory lecture related to this course. In the next lecture, we are going to review some of the important heat and mass transfer, fluid flow and you know, as well as thermodynamic background, and we will have a quick discussion on the different aspects of the major or the key equations that are involved in all those processes or transport phenomena. Thank you. I hope you liked this lecture today.