Research Methodology
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Lecture - 51
Theoretical Research: Mathematical Models of Physical Systems

Out of the various things that a theorist does, one important component is to obtain mathematical models of physical systems. Why do you want to do that? Basically, we want to do that because, having a mathematical model allows us (a) to understand the phenomenon, (b) to predict how the system will behave under different circumstances and (c) to test whether our understanding of the phenomenon is correct or not by making predictions and testing the predictions.

So, all these are possible if we have a mathematical model of the physical system.

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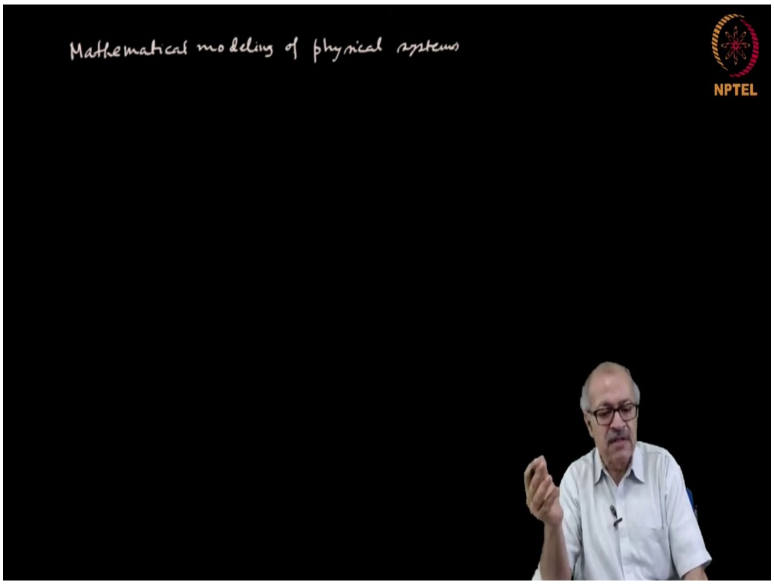

So, this is what we will study today: mathematical modeling of physical systems. Physical systems does not mean only systems coming from physics, it means anything in physical reality. In the method of obtaining a valid mathematical model of a physical system there are few steps to be taken.

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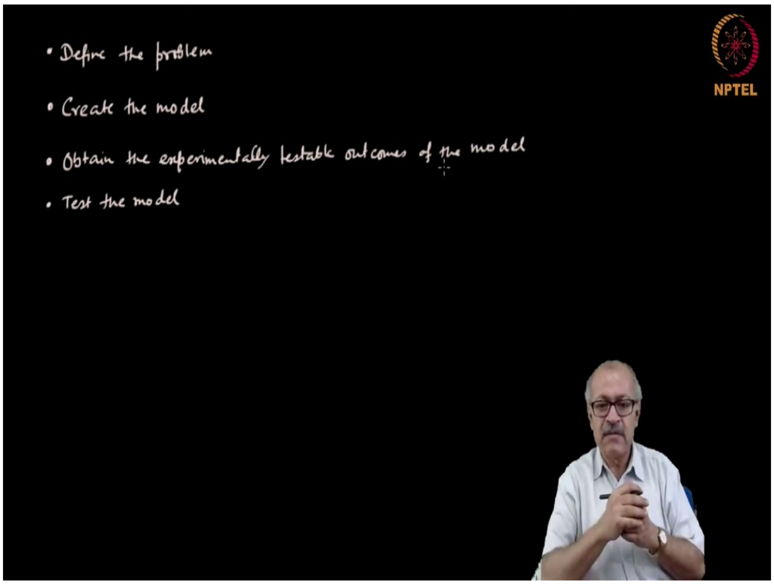

The first aspect that we have to talk about is to define the problem. What do you mean by defining a problem? Basically, identifying the phenomenon to investigate, identifying the various factors that may influence the output or the event that we are investigating.

Within that, there would be some which are independent variables, there would be some which are dependent variables: identifying them, separating them out. Then, apart from the variables, there would be the parameters of the system. These have to be identified. And then, to decide what the model aims to achieve, and accordingly the model has to be formulated.

I said that there are some variables which would be the dependent variables there are some variables would be independent variables. There are also variables and parameters. What are these?

If it is a dynamical system, something that changes with time, then there will be some variables that change with time. Now, these variables change depending on certain parameters. For example in a simple pendulum, the angle is a variable, but the length of the cord is a parameter. So the variable varies dependent on the parameter.

The parameter can be, or sometimes the parameter is also considered, as independent variable, because you might be able to vary the parameter independently of other things. If you are trying to model, say, the interior dynamics of a star like the sun, then obviously the variables would be the surface temperature, the core temperature, the constitutions of the core—how much hydrogen and how much helium are there and things like that—which will influence how much heat is generated, and thereby how much convection currents will happen. So these are the parameters.

In case of a planet going around the sun, the position of the planet in the elliptical orbit is a variable. The mass of the sun, the mass of the planet, the distance from the sun to the planet—these are the parameters. So, this way we have to identify the parameters and the variables. And if we identify all possible parameters that might influence the outcome, then that often does not really help in solving the problem. Why? Because there maybe too many parameters.

So, one also has to figure out which parameters are relatively unimportant whose influence is relatively lesser and thereby we can, at least initially in the initial phase of the modeling process, ignore them. We then state certain assumptions. The assumptions are that these have relatively minor effects and therefore, we initially ignore them. And then, later if we find that the model that we have created is insufficient to capture the phenomenon that we are talking about, then these have to be included.

So, these are the issues that go into defining the problem. When we talk about creating the model, we essentially create some kind of a mathematical relationship between the variables and the parameters. If it is a dynamical system we have to obtain differential equations, because, say, x is a dynamical variable, then we are asking how does it vary with time. So, dx/dt will be related to something in the right hand side. That is what you have to write down.

If it is some static phenomenon, for example, if you have produced an alloy, the ductility, the strength and other things of the alloy will be dependent on certain parameters. The composition of the alloy, the different metals going into it, the process, the temperature and other things that contributed to creating of the alloy—all these will be the parameters.

But then it will not lead to a differential equation. Rather it will lead to an algebraic equation. So, we have to identify whether we create an algebraic equation or a differential equation. After we have created the model, then we have to figure out whether the model is correct or not. In this case the model itself will take the place of whatever we have talked about regarding hypothesis.

That means, the model will have some experimentally testable predictions. That will need to be tested, and on that basis we have to figure out whether we are satisfied with the model or we have to improve the model. So, the next step is to obtain the experimental testable outcomes of the model.

Then we have to actually test the model. That means, we have to set up some experiment or observation, which will test whether these experimentally testable outcomes are true or false. And as we have said earlier, if they turn out to be false, we know that we have to improve the model. If they turn out to be true, that does not immediately say that the model is good. But that might indicate in which direction model has to be improved.

So, this is essentially the way of deriving a model of a physical system. These are the steps. I will illustrate these steps with an example. But in creating the model, often a clue comes from some experimental result. And the experimental result might establish some functional relationship between the independent variable and the dependent variable, and if such functional relationship is available, it should be made use of in formulating the model.

How to obtain that? That we have already done, therefore, we are not going into that again. Let us illustrate the process of model building using a very simple example, which, sort of, exemplifies the process.

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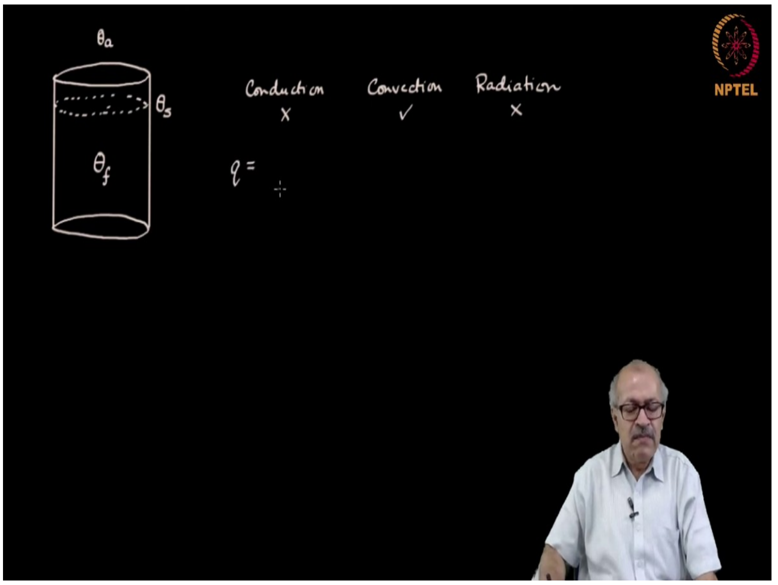

Suppose I have a cylindrical container, something like this. This is the cylindrical container which contains hot water, and we are trying to figure out how would that water cool down. So, there will be an average temperature of the water. The temperature at the top will not be the same as the temperature at the bottom. So, we talk about the average temperature. Let us call it theta in the interior of the fluid theta_f. And there would be the surface of the water. There would be temperature of the surface and there would be some temperature of the air.

Now, you notice that there are three mechanisms of loss of heat; the conduction, conviction and radiation. Now, by inspection of the system, we have to figure out which one will be dominant and which one would be of relatively less importance. And you would notice that in this case, since the air is a bad conductor of heat, so, the conduction from this surface to the air will be relatively less. So, we will say that this can possibly be ignored.

Similarly, unless the temperature is too high, the radiative heat transfer into the air would be rather small. So, these two are relatively smaller than this quantity. So, the convection from the bulk of the water to the surface and then from the surface to the air: that will be the main method of heat transfer. So, then that will be stated as an assumption.

But this assumption could be wrong, could be erroneous, and after we have formulated the model, we will test it against experiment. If it differs from the experimental results then we know that some of these, either one of them or both of them will have to be included in the model.

In that case we make the assumption that these two are initially ignored and we only root on the convection process. Suppose q is the heat that goes from the fluid to the surface and then the same amount of heat goes from the surface to the air.

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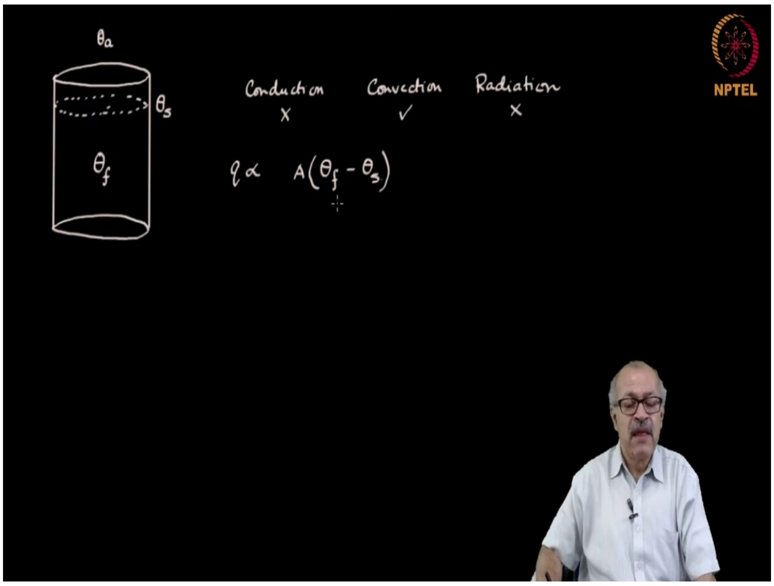

So, that can then be written as q, which is proportional to what it would be dependent on. Firstly, it will dependent on the area, A, times the difference of the two temperatures. The amount of heat that goes from the fluid to the surface is dependent on the theta_f minus theta_s (surface). Then, if you want to express that as an equality, we will have to put some coefficient.

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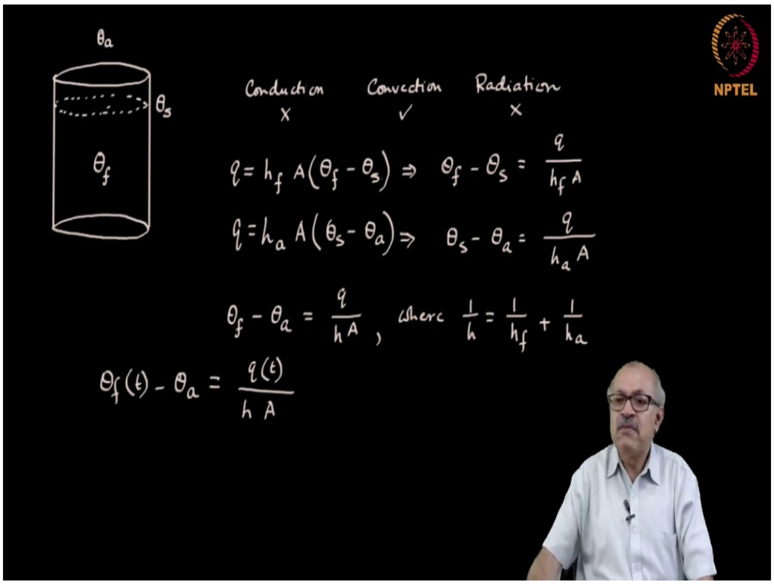

Let us call it the heat transfer coefficient h_f from interior of the fluid to the surface of the fluid. Now, the same amount of heat goes from the surface to the air and its heat transfer would also be convective. So, its character should remain the same, but the same amount of heat goes. Therefore, I have to write q itself and it will again be dependent on the area, this time it is theta_s minus theta_a, and it will be a different heat transfer coefficient. Let us call it h_a.

$$q = h_f \, A \, (\Theta_f - \Theta_s) \qquad\qquad q = h_a \, A \, (\Theta_s - \Theta_a)$$

So, we are actually proceeding by using common sense. We know that it will be dependent on the area, and it will be dependent on the temperature difference. Similarly here also it would be depend on the area and the temperature difference. We are simply writing in this way.

Now, from this, we can obtain theta_f minus theta_s is equal to q by h_f A and from this we obtain theta_s minus theta_a is equal to same q by h_a times the area. And then, if we add these two equations, we eliminate the theta_s and thereby we get theta_f minus theta_a. theta_f minus theta_a will be q by: well let me write a combined h times A.

$$q = h\,A\,(\Theta_f - \Theta_a) \qquad\qquad h = \left(\frac{1}{h_f} + \frac{1}{h_a}\right)^{-1}$$

Now, we can see that this will be 1 by h_f, this will 1 by h_A, which we are equated to 1 by h. So, we can write where 1 by h is equal to 1 by h_f plus 1 by h_a, or h is equal to this inverse; it is easier to write it this way. So, if you have obtained this, then we have taken a step in writing the differential equation, because one step, I said, is to figure out what are we trying to achieve.

We are trying to figure out how will the temperature of the water change with time. Therefore, whatever we have written as theta_f is not really a constant, it is a function of time. So we have to write theta f as a function of time. But theta_a, the air temperature for that period of time, we will assume that it is a constant. Now here the q, the amount of heat that goes, depends on the temperature difference. Therefore, it will not be a constant. So, this will also be q(t). h times area: these are the things that do not change.

So, we have obtained some kind of a relationship between these two variable quantities.

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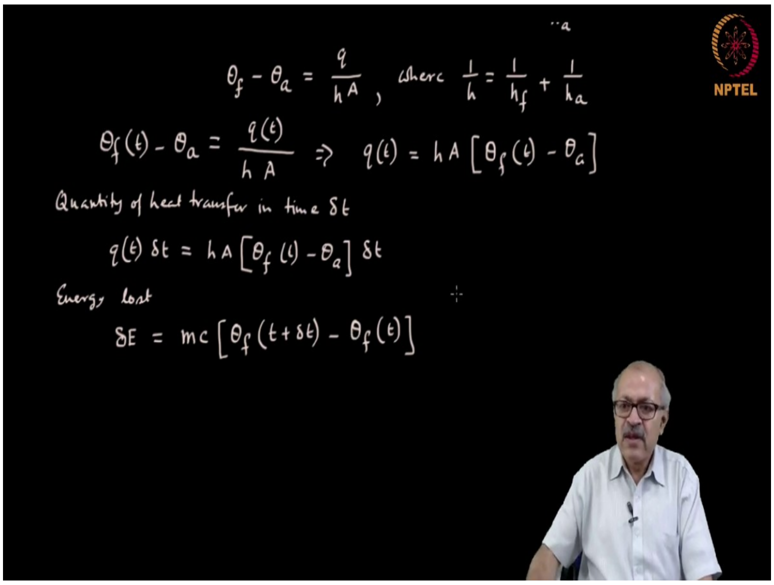

Now, let me write it this way. Let me write q(t) in the left hand side, h A times this theta_f as a function of t minus theta_a not a function of time. Now, notice that this is the amount of heat that gives the rate of heat transfer.

$$q(t) = h\,A\,(\Theta_f(t) - \Theta_a)$$

But suppose I now consider a small amount of time, say delta t, then the amount of heat that goes in the time is delta t. So, the quantity of heat transfer in time delta t will be q(t) times delta t. And if you have to multiply delta t in the left hand side we have to multiply in the right hand side also. It is h A theta fluid as a function of time minus theta air times delta t. Now, this is an equation obtained by considering the way of heat transfer.

$$q(t)\delta t = h\,A\,(\Theta_f(t) - \Theta_a)\,\delta t$$

But we can also talk about the amount of heat transfer. We can also talk about the amount of heat transfer from the point of view of the fluid. The fluid was there, it has lost heat and thereby it has reduced in temperature. And if you look at it from the point of view of the heat, the energy lost, from the point of view of the fluid, the energy lost will be delta E.

$$\delta E = m\,c\,[\Theta_f(t + \delta t) - \Theta_f(t)]$$

Let us represent by this: delta E is the energy lost, is m c the change in temperature. The change in temperature of what? Theta_f at time t plus delta t minus theta f times t. So, this will be the amount of heat that is transferred. This was larger, this is smaller, but this whole thing will be a negative number, because it is a loss of heat.

These two quantities, this and that, should be equal because this talks about the amount of heat that is transferred and this also talks about the amount of heat that is transferred. So, they should be equal, so let us equate the two right hand sides.

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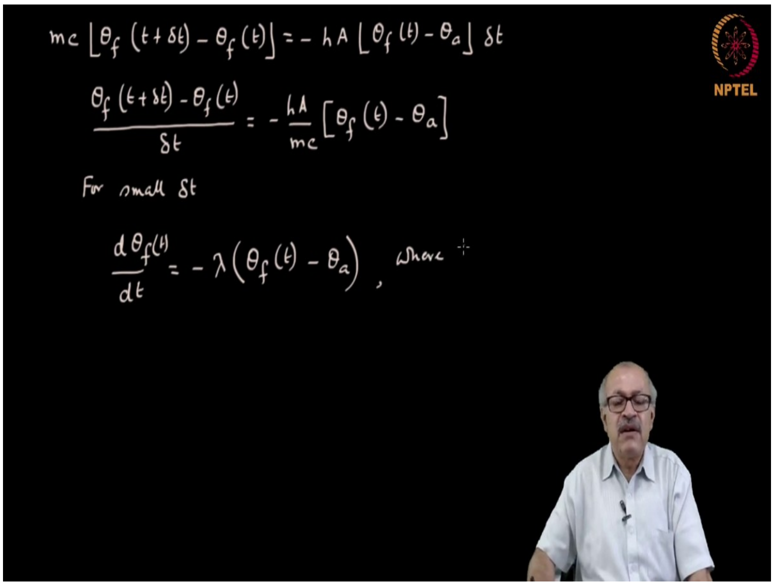

If you equate the two right hand sides, then we get m c theta_f t plus delta t minus theta_f t. So, this is the amount of heat that goes. Now, this is a heat loss, therefore, this also has to be expressed as a heat loss. So, we have to write it as: equal to minus h A theta_f t minus theta_a delta t.

$$m\,c\,[\Theta_f(t+\delta t)-\Theta_f(t)] = -h\,A\,(\Theta_f(t)-\Theta_a)\,\delta t$$

or

$$\frac{\Theta_f(t+\delta t)-\Theta_f(t)}{\delta t} = -\frac{hA}{mc}(\Theta_f(t)-\Theta_a)$$

Now, let us bring the delta t here and the m c here. So, we have theta_f t plus delta t minus theta f t by delta t and in the right hand side it will be minus h A divided by m c and here it is theta_f at t minus theta_a. So, this way we have written down an equation that almost looks like a differential equation. The only thing now is that, if this delta t is small, then this is actually the derivative of theta_f with respect to t.

So, for small delta t then this becomes d theta_f/dt, this is the definition of the derivative. Let us call this lambda times theta_f t, so this was also a function of t minus theta a.

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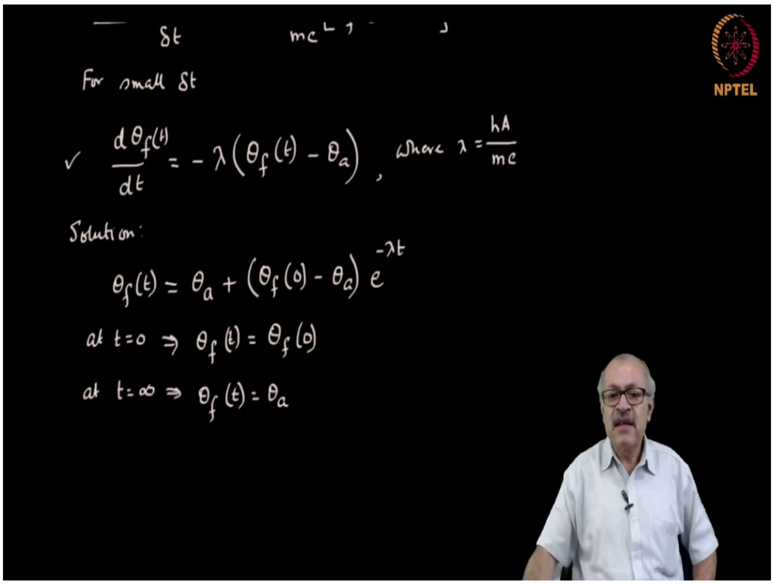

$$\frac{d\Theta_f}{dt} = -\lambda(\Theta_f(t) - \Theta_a) \qquad \text{where } \lambda = hA/(mc)$$

So, here we have a differential equation: a differential equation which talks about how would theta_f, the fluid temperature, change, where your lambda is h A by m c. So, we have a differential equation here. This is a differential equation that we have obtained. This is then a model of the system that we are trying to capture.

We are trying to understand how would the temperature of the water change with time and solving this differential equation we can get that. So, after having obtained it, remember that this is under the assumption that conduction and radiation would be much smaller than the convective heat transfer. Under that assumption this has been obtained. Now we have to check whether the assumption is correct or not.

I have already stated the steps in the process of formulating a mathematical model is to find out what is the experimentally observable prediction from the model. That can be obtained in case of differential equation by solving the differential equation. Now, I will not actually solve the differential equation because this is not a differential equation solution course. This can be solved by the integrating factor method, but I will just write down the solution.

$$\Theta_f(t) = \Theta_a + \left(\Theta_f(0) - \Theta_a\right) e^{-\lambda t}$$

The solution is theta_f of t it will have to be expressed in terms of the fluid temperature at the initial time. This will be theta_a plus theta_f at the initial time 0 minus theta a then multiplied by e to the power minus lambda t. That will be the solution.

Now, a quick check first. Any theorist will do a very quick check to see whether we are on the right track or not. How? Simply by putting t is equal to 0 and t is equal to infinity. So, at t is equal to 0, this becomes 1. And therefore, theta_a minus theta_a so that gives theta_f at 0. theta_f(t) becomes equal to theta_f at 0, which is right. At t is equal to infinity, this becomes 0, therefore, the whole term becomes 0. And what remains is this, so theta_f(t) is equal to theta_a. So, after infinite time the temperature of the fluid becomes the same as the temperature of the air, which is also right. Follows from common sense.

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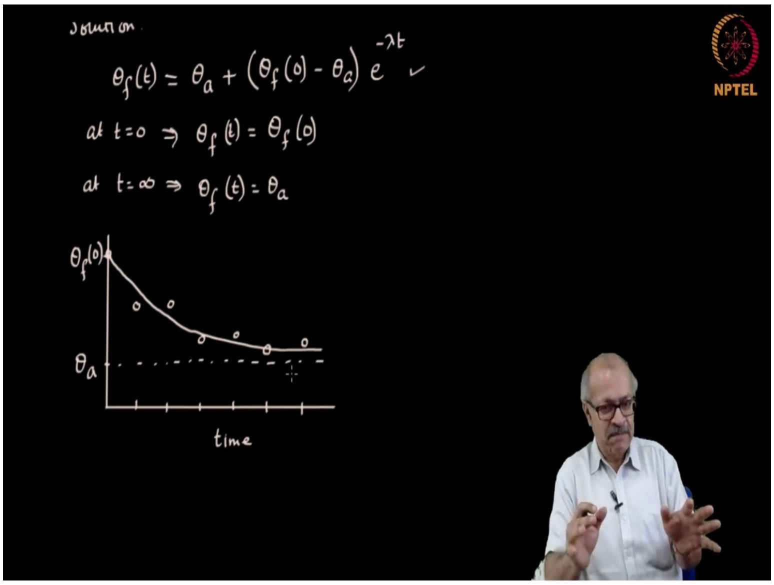

So, it is clear then that it will follow a graph. The reduction of temperature will follow an exponential curve, which will start from theta fluid at 0 and here is theta a. So, it will go up to this, it will fall up to this. So, it will fall like a exponential decay, following this equation, which I just wrote.

Now, the last step is to check whether we are on the right track or not. How do we check? We will perform an experiment. That means, we will fill a glass with hot water and then we will have a thermometer dipped there and we will measure the temperatures at different times.

Suppose, I get values something like this. I can also take a reading at the initial point; it may be somewhere here. Is it satisfying our prediction? You see that now these are actually different from the actual predictions. The question is then: are the differences due to random errors? If you look at the difference, does it follow the character of a random variable or is there some systematic deviation?

If there is a systematic deviation, then you have to talk about including the factors that were initially ignored. How do judge? Well we have already learnt that this can be judged by the chi square method. This can be judged by various possible techniques that we have learnt already. So, using that, we will figure out if the differences follow the character of a random variable. If so, we know that we are on the right track, the readings could have those random fluctuations.

But if we find that it does not follow the character of a random variable, i.e., the probability of getting that chi square value is less than 5 percent, then we will say that, no, there is something else. We will need to include some other factor that we initially ignored. So, that is the method of obtaining a mathematical model.

We have shown a very simple situation, but this is a representative situation. In research, you would encounter more complicated situations to model, more complicated phenomena to model, but effectively the method remains the same.