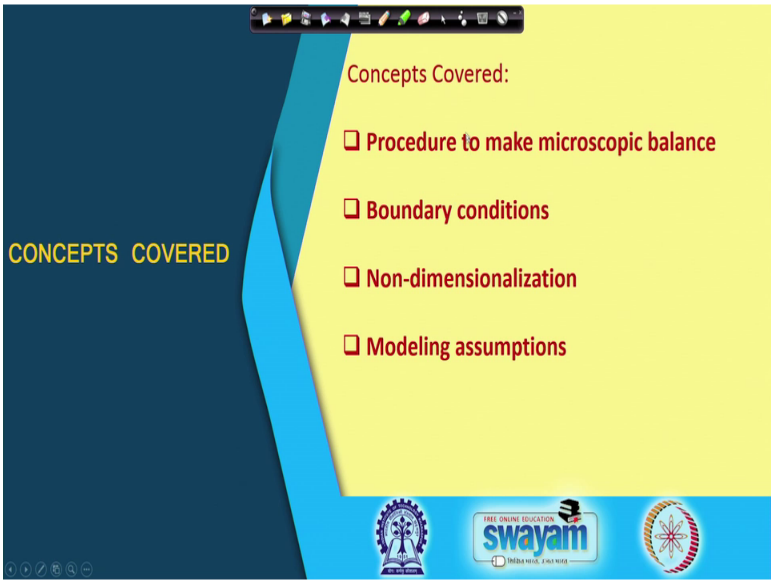
Mass, Momentum and Energy Balances in Engineering Analysis
Prof. Pavitra Sandilya
Cryogenics Engineering Center
Indian Institute of Technology, Kharagpur

Lecture – 26
Microscpic Balance Equations – III

Welcome. In this lecture, we shall be continuing our previous analysis for the microscopic balances. We have learned so far what are the 3 ways for microscopic balances in the term of the conservation laws mass balance, energy balance and momentum balance. Now we after we obtain these equations we should also have some idea that, how to go about implementing these balances in a real life situation. So in this case, we have to follow certain procedure in a step by step manner so that, we can arrive at the right equation to which represents the particular process under study. And these equations it may be single equation or it may be multiple equations depending on the situation and these equations are also called the modal equations.

(Refer Slide Time: 01:23)



So in this lecture, we shall be studying these following that to procedure to make the microscopic balances for a given system. And whenever we are making some balances to solve the problem, we have to also prescribe some initial conditions some boundary conditions because, any kind of problem we will find that we will have some starting point and we generally like to trace that how that particular process is progressing with time and what are the changes happening in the process. And another thing is this, what are the conditions, which are there at the boundaries of the particular system because, that boundary conditions would dictate the internal features of a process. For example, suppose there is there are 2 walls and these 2 walls are the you can say that these 2 walls are inclosing a certain room ok.

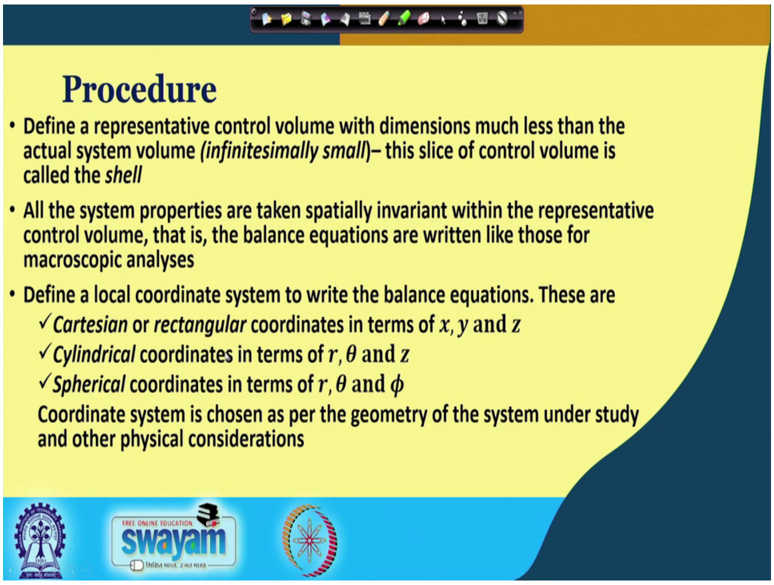
Now, you can see that depending on the temperatures at the 2 walls, the room temperature will be decided. That means, for the wall temperatures or the boundary conditions and they are dictating the inside condition of the room and all this things are taken care of whenever you are designing any kind of say air conditioner, you we have to consider all the conditions at the outside the room and accordingly you decide that what kind of air conditioner, you will select.

So similar kinds of example, you will find that in our nature that wherever we are finding that the conditions at the boundaries are dictating the features within a particular system and that is why we it is very important for us to judicially select the boundary conditions. Wrong boundary conditions will lead to wrong interpretations of the actual the realities, then comes the non dimensionalization, this particular thing pertains to the solution of the equations that the microscopic balance equations. We will find that why we need to non dimensionalize them so that, we can make the solutions more general and at some sometimes, we make the solutions easier to handle.

So, we need this particular step and lastly the modeling assumptions because, even though all the microscopic balances, which have been derived and shown to you are in three dimensional unsteady state. But many situations arise where you find these need not solve this whole 3 dimensional and unstructured solution may sometimes, we are talking about steady state and sometimes the process is such that the variation of the particular scalar filled in any particular direction may be neglected in that way, we can reduce the dimensionality of the problem. And it may so happen that we can reduce the 3 dimension problem to a simple one dimension or even if we assume a steady state, we find that a that kind of a unsteady state say 3 dimensional equation reduce to a single or a multiple number of ordinary differential equations and this kind of assumptions lead to a more approachable solution more practical solutions of these various processes.

So, what kind of assumptions we should make and under what basis, some basic ideas will be given to you and you will find that in actual life, there will be many instances, where you have to, you have this whatever I am going to teach you that may form some basis to you to decide that how to tackle the real life problems.

(Refer Slide Time: 05:15)



Now, let us come to the procedure ok. So, when as we have set earlier also that whenever we are going to analyze a particular system, we first need to figure out that what is the area or the domain, which is going to be studied. So, we are not going study everything we fix a particular domain and we focus our attention on that particular domain and write all the balance equations as per that domain.

So, what we call this first we have to select a control volume, we should to be representative of the actual system, it should not be the control volume does not represent the system the whatever is happening in the actual system the control volume, you can say is just a smaller way or miniaturization of the whole space.

So in the space, we are selecting a and the subspace with the whatever is happening in the whole space, we will also be seeing within that subspace. So that is why, we are saying that the control volume choice has to be made very discretely. Now these control volume should be infinitesimally small; so that means, is should have the dimensions of the control volume should be must less compared to the dimension of the whole system, because in the microscopic balance we are trying to figure out the distribution of particular scalar field within the system ok; that means, you want to find out the profile of the scalar fields like temperature profile, the construction profile, the velocity profile, etcetera.

So for that, we have to go as much as possible point by point, but in practicality in reality the point we cannot make a point balance ok. So, we always chose a small domain which will be having enough space. So, that we can make the balances, but it should have a dimension which is much smaller than the dimension of the whole system so that, we can make the appropriate balances.

So, this particular control volume is sometimes called the shell. So many times, we will here in the literature the shell balance. So, whenever you are encounter this word shell balance it basically, it means that you are making a taking a small control volume and over which you are going to make all the balance equations.

Now, whenever you choose a control volume because, we are interested to find the profile; that means that we want to know the variation of particular scalar field point by point location by location. Now, you see that whenever we are choosing control volume small control volume, if we say that we may question that within the control volume, there could be a distribution? Yeah it is possible, but point is this the way we are directed to find put the control volume we say that it should be must smaller, it means what that the within the control volume we assume, there is a proper distribution or uniform distribution of any of the properties and you will find that as you found in the derivation of the microscopic balances.

There also we started with a control volume say for example, in (Refer Time: 08:38) coordinate the control volume has a volume of delta x, delta y, delta z and this delta x, delta y, delta z were having finite dimensions, but when we derived when we are ultimately derive the balance equations, what we did? We put these delta x delta y delta z tending to 0; that means, we are making very very small ok.

So, when you make them very very small. So, it is assumed that the particular scalar field will be having a same value over the entire control volume; that means, each control volume is taken to be a well mixed system and then when we take the limit of the delta x, delta y, delta z to 0, we are kind of reaching a point location that is how we are going to find out the profile of the scalar field.

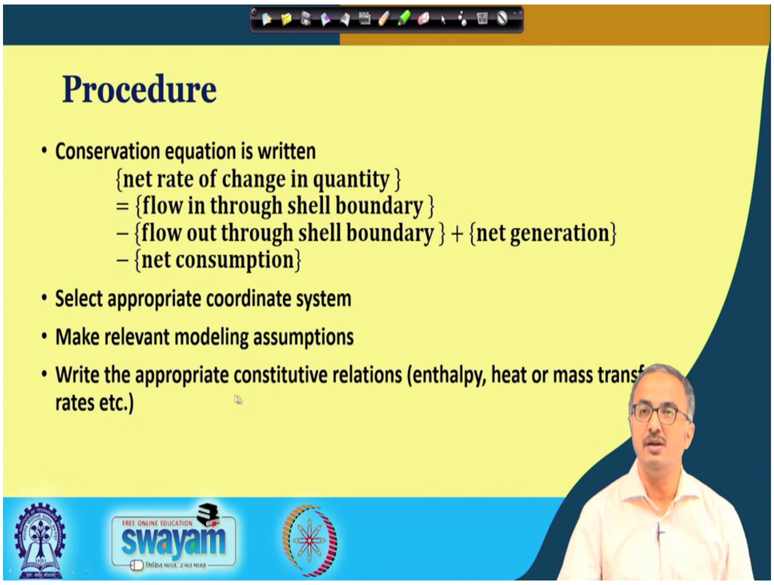
Now once, you make the profile of the scalar in the scalar there is in that particular control volume. Now volume the whatever, we learn earlier also in the microscopic balances the similar kind of theories will also be applicable for the microscopic domain. Now after that we need to define some local coordinate system and as I told you in my earlier lecture that, we derived the microscopic balance equations for different types of coordinate systems and as I told you earlier that the proper choice of the coordinate system eases the solution of the particular balance equation or equations.

So, it is very very essential for us to choose the proper coordinates system. So, as we have said seeing that we have 3 types of coordinate systems, one is that Cartesian or rectangular in which we represent in terms of x, y, z and then we have the cylindrical coordinates when which is represented by r theta and z and spherical coordinate that is represented by r theta and phi.

So, all this things quite are known to us and coordinate system should be chosen as per the geometry of the system. For example, if we have a cylindrical vessel the first choice could be that we go with a cylindrical coordinate, but again you will find when you choose a cylindrical coordinate with some assumptions, you see that the particular coordinate system may get reduced to a rectangular system that may happen ok, but the first choice would be that if the cylindrical the system is cylindrical say for example, we have a reactor; obviously, cylindrical column.

So for that, we may choose at the first time that it was a cylinder cylindrical coordinate system ok. So in that, case we may choose rectangular, but you will find the manipulations the things we search that a geometry of this particular cylinder will make the choice of the rectangular coordinate systems a bit more involved ok. So in that, we can see that the geometry of the particular system at hand will be dictating the choice of the particular coordinate system.

(Refer Slide Time: 11:55)



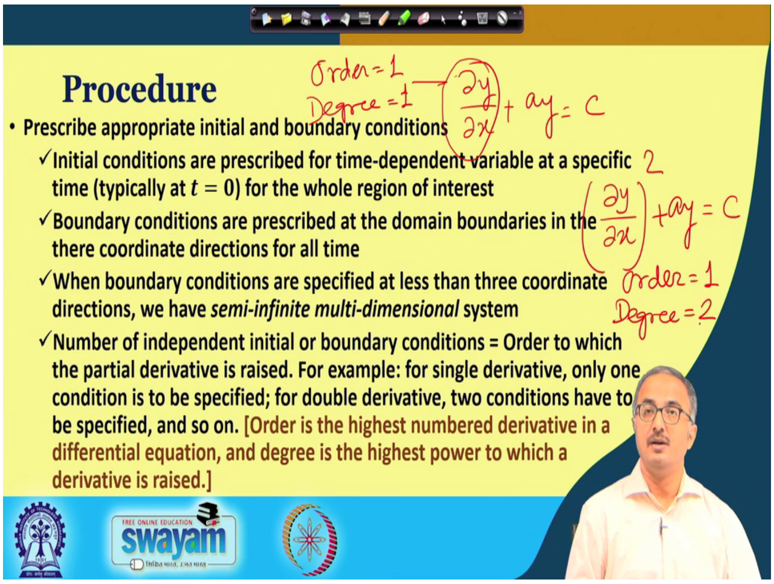
And then we once we do this all these then we go to write the conservation equations and this is the general conservation equation that net change rate of change of any quantity is equal to flow in through the shell boundary, then minus flow out plus semi shell boundary plus some net generation and minus some net consumption.

So, this is about we have seen earlier. And this particular is conversion equation should be kind of remembered, because even if you are forgetting something here and there during your solution, if you remember this basic theory concept, perhaps you can derive many of the equations right on the spot. Then after selecting the coordinate system make the relevant modeling assumptions and I will talk about the assumptions later on and then after see model equations are based on the some conservation laws.

Now that is not enough, you will find and we have seen that also when we are doing the microscopic balances in that we found that even after writing the model equations there were some parameters, they were not coming automatically from the balanced equation for example, the density for example, the specific heat that for example, the heat transfer coefficient. So, these parameters are not coming automatically naturally from the model equations.

So, to estimate these values again we need some other equations in terms of some correlations in terms of some tabular data. So, all these things come we call that constitutive relations. So, we need the constitutive relations after we set up the balanced equations from that we figure out which are the parameters, which need to be estimated to solve the balance equations. So, we need to find out the appropriate constitutive relations for example, we find enthalpy heat or mass transfer rates etcetera ok.

(Refer Slide Time: 14:06)



Now, then we have to after getting the model equation then the constitute relation now before we solve now you have to prescribe the initial conditions and the boundary conditions, initial condition means that the state of the process at a given time is prescribed and that time is generally taken to be 0, there is no zero time as such, but whatever the starting point is taken to be 0 and then we progress with time and then boundary conditions as I told you that at the boundary do boundary of that particular domain of study, what are the various conditions and I will talk more about the different types of boundary conditions possible for a process system.

So, as I told you that initial conditions are prescribed for time dependent variable at a specific time typically at t equals to 0 for the whole region of interest; that means, the initial condition will be applicable both for the boundary as well as within the system and then we have a boundary conditions, which are prescribed throughout the boundary of the system only and again these are for all the time ok.

So, this is the difference between this initial and the boundary condition and sometimes, you will find that even though I am telling you that initial condition is for say time, but many a times even in space we find that the special coordinate, where is like time for example, you have a steady state problem and one dimensional problem in that case you see that suppose, you are going from your home to say your college ok.

Now, you see that suppose your you have a one dimensional movement ok. You are not going anywhere one dimensional movement, I can approximate your movement from your home to college one dimensional system and suppose it is steady state; that means your going to a constant speed ok. Now you see that the starting point is your home and the ending point is your college, now in that case what you find? College or office, it could be now you find that that when you write the balance equation for this it may reduced to only a one single special direction.

So, this will give you a an ode ordinary differential equation and when you want to say you get something like say some your any kind of what you call it you want to know the speed etcetera, in one dimensional you can write the equation and then you find that when you put this, you find that the particular this particular space that like if you use a space given by is x, x is direction of your movement then this particular x may be suppose, you are measuring a temperature along the along your root ok.

Now, this temperature variation along your root is one dimensional and then you find that your getting some equation, which is one dimensional and in that case you find that that the first that the you start that are you start the temperature measurement that your home and then perhaps you are measuring temperature along your root. So, the first temperature which you are prescribing at your home is a initial condition.

Now, you see the even though physically it is a special dimension, but mathematically you find these becomes like an initial condition ok. So, mathematically it is different mathematically, it is like an initial condition even though specially, it is a boundary condition. So, you start like this that that the as if your replacing time by x ok. So, you put at x equal to 0 temperature is this. So, understand that many a time the special coordinate mathematically behave like a temporal coordinate, but in reality it is not so ok.

So that is why, you will see that as you go along doing this kind of modeling, you will find that many situations arise ok, then what happens by this kind of means mathematical interpretations, you find that the solution procedure becomes quite generalized, you do not have to invent different procedures for different means boundary type condition, initial type condition because mathematically does not matter the we look at the type of the equation after writing the balance equation that will decide that will decide solution procedure ok.

So, that is what I wanted to tell you about the initial condition and the boundary condition you should not be thinking that initial condition must be having time unit, it may have space unit also mathematically not physically when boundary conditions are specified at less then 3 coordinate directions then we can say that we have some semi infinite multi dimensional system.

Many a times, we neglect the boundary effect ok, maybe if the boundary is too far of we can say that effect is not filled within that system is the core of the system ok, then in that case what happens we can say that as if it is independent of the boundary conditions, it happens in many systems you as we go along we find many system, I will give example to you to tell you that how a actual 3 dimensional system may be reduced, but by considering and the infinite dimension in one particular direction and reduce it is spatial coordinates ok.

So, these are what we call the semi infinite, it is not infinite semi infinite because, we are still retaining the variation in one or two directions. So, we are not trying to solve for all the 3 directions and then whenever we are talking of these boundary condition initial conditions, how do we decide that, how many numbers of initial conditions is to be provided, how many boundary conditions are needed? So, this is very simple for you to judge, you will see that number of any that any independent initial or boundary conditions is equal to order to which the partial derivative is raised.

Now, order and degree perhaps you know let me just recapitulate for you that order suppose, I have a something like d dou y by dou x plus a y equal to say C ok. So, this is a first order equation ok.

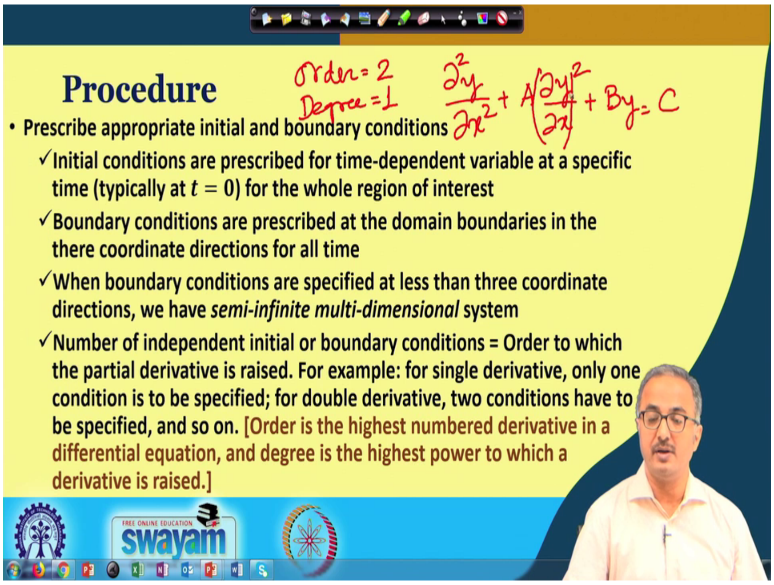
So, you see that you see the highest deri highest derivative we are doing ok. Now suppose, I write the same equation like this dou y by dou x whole square plus a y is equal to C. Now in this case, the difference is what the order still remains 1, but the degree is now 2 here, the degree is 1, here degree is 2 this is order 1 and degree 1 and here order is 1 and degree is 2 ok.

So, this is the difference between the order and degree. So similarly, if you haves so let us write a second order equation.

Student: First one that.

Now let us write another equation which is of say order to ok.

(Refer Slide Time: 22:00)



So, let us see like this dou 2 y by dou x square say sub some dou y by dou x plus say B y equals to C. Now in this case you just see that what is the highest degree of derivative here? You see the highest degree is 2. So, this order is 2 ok

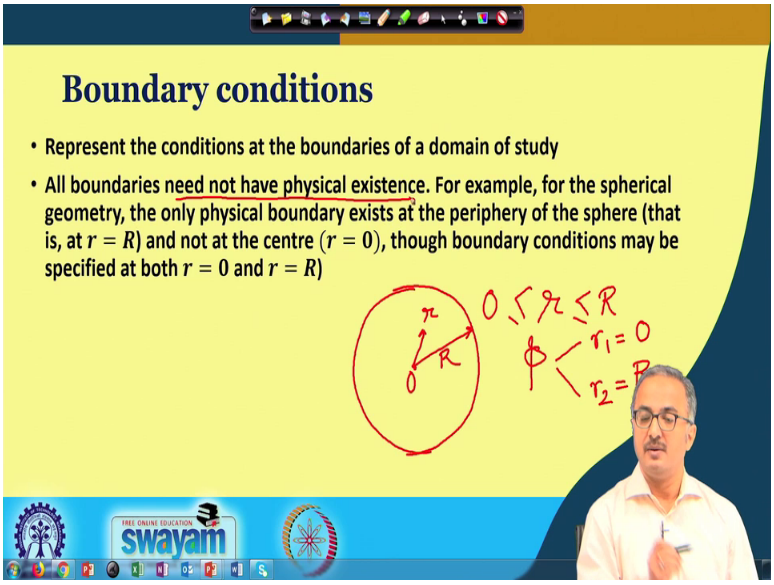
Now, if I say what is the degree of this equation? Now again, you to see that 2 these degree is the power to which this particular equation is have the highest power is there as produce here again 1 ok. So, degree is 1 ok. So, I hope that you can understand how we decide the order of an equation and the degree of an equation ok. So suppose these goes to a square.

So, order still remains the 2 ok. So, this you should be very careful. So here, what we are saying about these that the number of the number of independent initial or boundary condition, this word is very important that in therefore, they will be independent there should not be dependency of the initial and boundary condition each other, if they are dependent then; that means, we are over specifying the things ok.

So, we do not should not word specify anything. So, there may be independent initial or boundary conditions equal to order to which the partial derivative is raised. For example, like if we have a single ordered single derivative single order; that means, only one condition is to be specified for double derivative, we have to respect two conditions.

And generally you will find that the derivative in the time direction is generally one sometimes we get 2, but generally it is one, but for the space derivative we will find that we get both type of things, whether we get both a single derivative as well as double derivative. Single derivatives are generally associated with some convective terms and double derivative are associated with the diffusive terms ok.

(Refer Slide Time: 24:26)



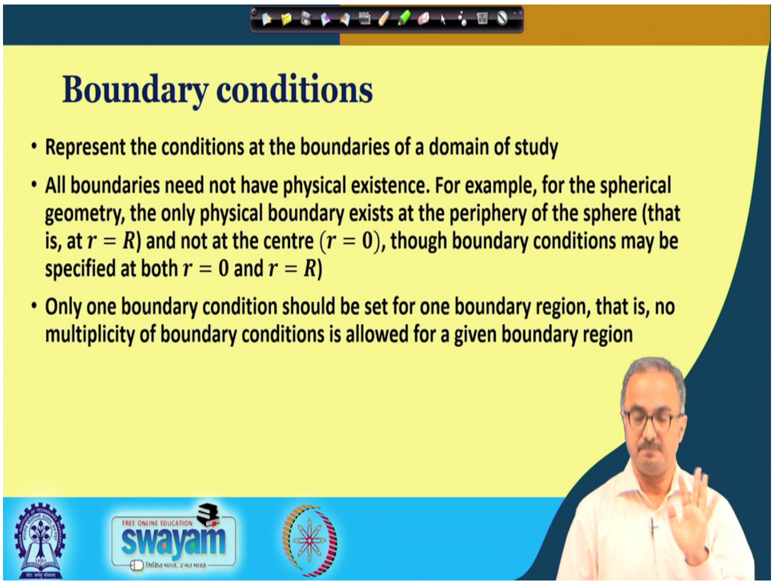
Now we come to the boundary conditions they as I told you that they represent the conditions at the boundaries at the domain of study. And all boundaries need not have physical existence, this is very important as I was telling the boundary does boundary is from the mathematical point of view ok.

Now, for example, I visual let us talk of a sphere, let us talk of a sphere. Suppose, this has the center and suppose the radius is say capital R and let us say that any redial position is given by a small r so; that means, r will be wearing between say this is suppose, this is the 0 origin between 0 and R. So, suppose we are writing some balance equations may be in terms of concentration, velocity or temperature.

So, what we generally do? That if we find that we have a second order equation, we find that we have to specify the value of the say this is the phi is the particular property for which we are solving it ok. Now this phi we has to be specify the boundary condition let us specify at to say r 1 and r 2 at 2 (Refer Time: 25:50) points. Now say, r 1 I choose because I have to solve within the whole spherical domain. So, I will choose this r 1 equal to say 0 and this r 2, I select as this particular periphery of the sphere.

So, I put this r 2 equal to R. Now you see that when I talk of r 2 equal to R it means what? That this is physical boundary I can see that ok, but when I talk of r equal to 0, this knows the physical boundary it is a boundary here, it is just a starting point we have taken. So that means, what the boundary conditions need not have any physical existence, they may their just it is kind of you can say some mathematical way of representation of the particular process, where starting point and the ending point. So, that is what it said that all the boundaries need not have physical existence ok. So, this is what I have shown you by this particular example.

(Refer Slide Time: 26:57)

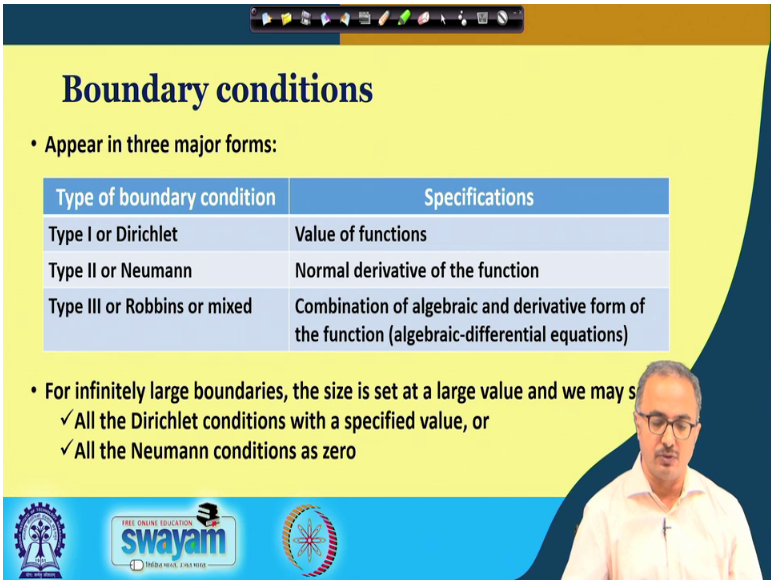


Now, only one boundary condition should be set for one boundary region, that is the there should not be multiple boundary condition for the same domain otherwise, it will you know there will be kind of a could be clash because, at a given particular location we have only one and one condition it control multiple conditions at one location.

For example, if you are saying that you there is suppose you are putting a pan with some kind of say water or milk on the oven. Now you see that you know that the when you putting on the oven and your, we are passing you are means burning this thing then what happened? The liquid inside the pan will started to heating up. Now boundary condition could be that, what is the temperature may be at the bottom of the pan or may be how much heat flux is being inputted through this bottom of the particular pan.

Now, you cannot prescribe both the heat flux as well as the temperature at the bottom because, if you keep one fixed other will have to vary to keep that first one fixed. So, if you want to keep the heat flux first the temperature as to vary and vice versa. So, you see that multiplicity of the boundary conditions is not permissible to define any kind of physical problem. So, you have to see that what kind of boundary conditions, you should have.

(Refer Slide Time: 28:30)



And now we see that there are various kind of boundary conditions in various systems, but all this boundary conditions again, may be classified into 3 basic types and here I am I am showing the 3 basic types of boundary condition. First what we call the type 1 or Dirichlet type. So, these are the names of the scientist who proposed this kind of boundary conditions ok.

So, type 1 is Dirichlet and this is when we are prescribing a value of the functions; that means, what it is suppose as I told you that in the pan your heating some liquid to prescribe the temperature at the bottom of the pan. So, that we call the boundary condition of type 1 or many times we call them Dirichlet condition ok. So, this way you can also finger out that suppose, you are starting a car form rest we say it is the boundary condition is that we can say that it is rest means it is type 1; that means, we are prescribing the value as of the velocity of the particular car.

Now, please understand that the when whenever we are putting the value immaterial of the time or boundary, boundary conditions it does not matter that we are whenever we are putting the value specified value we are calling it type 1 we are not giving any kind of derivative or other thing. Now when we go to type 2 or what we call Neumann condition here, we are putting some kind of normal derivative for example flux. So, your are saying that what is the say you are having a pipeline through which some liquid is flowing or gas is flowing, you are saying that what is the mass flow rate per unit area at the inlet of the pipe?

So, that is the flux. So, in this way when you are prescribing the flux that becomes the second type 2 boundary conditions with. So, any go to acceleration you want to propose that will be a flux boundary condition; that means any kind of derivative whenever you are proposing. Now when you understand this when you propose a velocity, velocity is a derivative if you are trying to find out the location ok.

Now, if you prescribe the acceleration that becomes the derivative, if you are trying to find out the velocity ok. So, you have to understand this; that whenever you are prescribing this you cannot say that see if am trying to find out the velocity profile to a pipeline, if you provide velocity then it is even though velocity is d x by d t, it should not be taken as the type 2 boundary condition.

It should be taken as type 1 boundary condition, but if you are prescribing the acceleration then it should be treated as type 2 boundary condition not type 1 boundary condition; that means, the scalar filed for which you are solving that particular balance equation, that value should be prescribed at the boundary to qualify as type 1 and that derivative should be considered if (Refer Time: 31:46) type 2 ok. Not any other variable, which may be derived or the derived from that particular actual variable or may be of that particular actual variable, which where solving for can be obtained from other variable ok. Not that way ok, you have to construct the particular variable which we are solving for that is very important us to know.

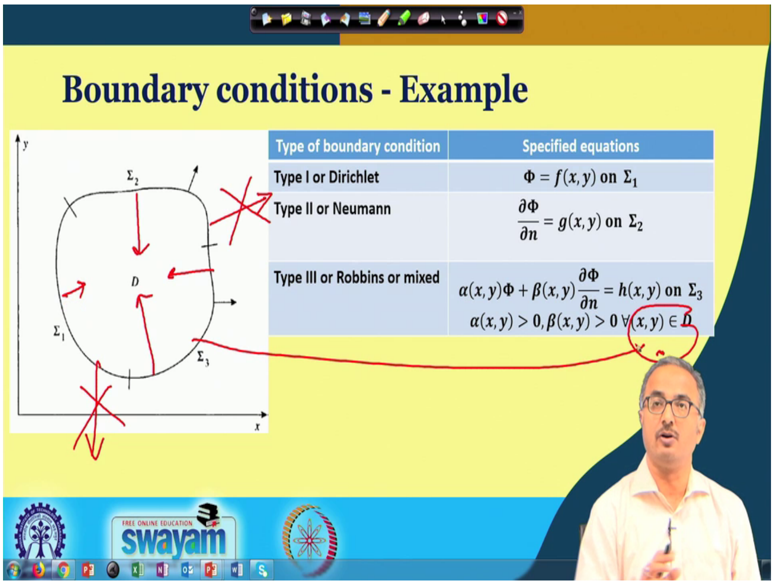
And then is type 3 boundary condition, it means the type 3 what we call Robbins boundary condition or mixed boundary condition. In mixed boundary condition, you have both the kind of mixture of both the type 1 and type 2 ok. So here, this will be liners to some algebraic differential equation and for infinitely large boundaries the size is set at a large value and we may set all Dirichlet or all Neumann as 0.

So, this is an another thing that whenever you have infinite as I was telling that we have saying infinite domain. So, we may; that means, size is set at too large because, infinite how to represent the infinite there is no way to represent infinite in means any kind of in kind of whenever you are going to make some kind of coding or something you put a large value.

Large value compare to the actual domain of your study that the dimension of domain ok. In that case, what you do either you put all the normal conduct should 0; that means, you say that velocity the profile for that you say that dou v by dou x or dou v by dou y or dou v by dou z to be close to 0 at the boundary ok. Or you say that the velocities are some constant and it is not that you to have prescribe only first order derivative, you may prescribe second order also; that means, you can put dou 2 v by dou x square as 0 or dou 2 t by dou z square as 0 ok.

So, it has to be some derivative. So, this kind of things also done mathematically to solve these domains; whenever we have some infinitely large boundaries.

(Refer Slide Time: 33:45)



And here, I have shown that if I take a 2 dimensional case here, I shown that how we apply this boundary condition to dimensional case we have. So, we see that we have taken all this with different kind of boundaries the sigma 1 is one boundary, sigma 2 is one boundary and sigma 3 is another boundary and D is the domain of interest of study ok.

Now, you see when we talk of type 1 or Dirichlet condition what we mean? We shall it prescribing see we are solving for some variable phi, may be temperature, may be velocity, may be something else. So, you may prescribing the phi value as a function of x y on the time sigma 1 ok. So here, we are prescribing this whole domain we are prescribing the value of the phi; that means, it determine constant or specified ok. It should not a derivative ok.

Similar thing goes with a similar conditions also in initial condition also, you should not when we say specified it should not be taken as constant value, it should be taken as a variable, but in saying case of initial condition we lead to the initial condition may be a function of space ok. So, it should not it. So, the constant similarly when we say this we say it v function of this x y, but should not be having any derivative.

In the second boundaries saying, if you talk of second this type 2 we can talk of this that dou phi by dou phi by dou n equal to some function on sigma 2. So, in this particular domain we are putting a type 2 kind of boundary condition and next is the type 3 suppose, sigma 3 what we are saying you can see now this particular equation here, we have these type 1 type and this is a type 2 type and again we are having these a combined boundary condition.

So, this is a differential algebraic equation and we say that alpha x y b x beta x y are more than 0 and this x y x y belong to this particular domain; that means, we are solving for x y not outer domain, but within this particular domain; that means, we always this particular thing means it means that we have to always travel inside ok, from any boundary we go you have travel inside. So, we cannot travel outside this is not permissible this not the that is the meaning of this particular thing that x y must belong to the domain of our study.

(Refer Slide Time: 36:15)

Student: (Refer Time: 36:15).

So, these are the few references in which you can find a very good position about the concepts and topics I have covered in this lecture and we shall be continuing this lecture for some more on the more on the procedure of these balance equations.

Thank you.