Multiphase Microfluidics
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Lecture – 07
Computational Techniques

Hello, in this lecture we will be talking about the computational techniques that can be used to model multiphase flow in micro channels. So, as this course is not predominantly on computational methods, and there is no prerequisite that one should have a basic understanding of computational fluid dynamics or other computational methods. So, we will first look at what computational fluid dynamics is, and then we will talk about what are the equations that are required to be solved for multiphase flows.

So, what we will be looking at that how our mathematical model can be formulated for modeling multiphase flow in particular with respect to micro fluidics.

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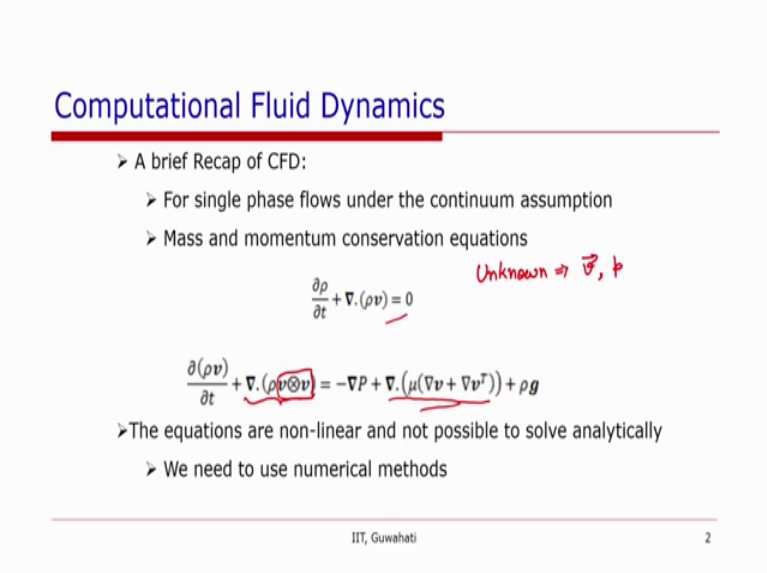

So, before we do that, let us looked at look at very briefly what computational fluid dynamics is. So, if we a look at single phase flow, the single-phase flow under continuum assumption can be modeled using navier stokes equations; which are momentum conservation equation, and mass conservation equation, and the fluid is Newtonian as you can see from this term.

So, the mass and momentum conservation equations in this; what we have as unknown is the velocity vector, and pressure they are our unknowns. So, we have 2 equations in the vector form you can say, and then we need to solve these equations for obtaining or to obtain pressure and velocity. Now because this equation is non-linear, the equation momentum equation, the convective term as you can see here is non-linear. So, it is not always possible to get a solution analytical solution for this partial differential equation. And we need to use some numerical method to do so.

Only under certain conditions, when we can eliminate or when we can linearize the convective term, under those conditions it is possible to obtain an analytical solution for this navier stokes equation.

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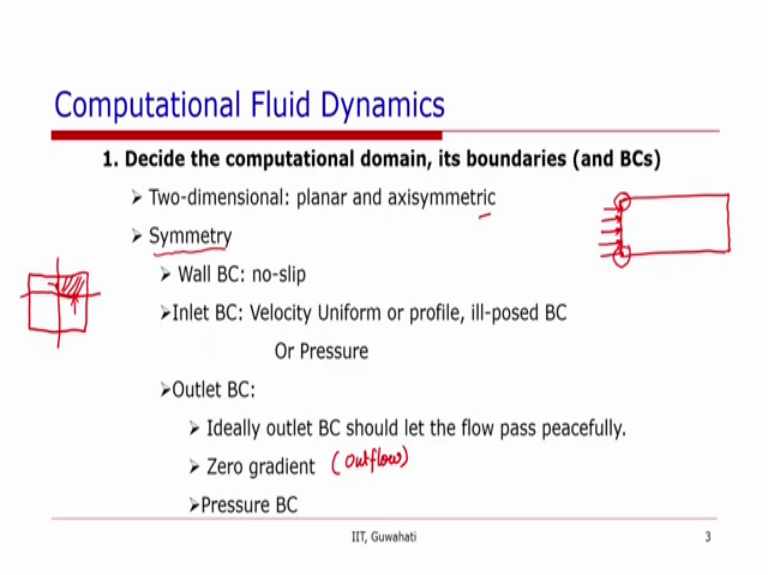

So, there are a number of techniques that can be used, or that have been used to solve navier stokes equations. We are just describing or I am just going to describe only one technique very briefly, to give you an idea what are some of the terms that we might be talking about later on so that you do not feel that you do not know those terms.

So, in computational fluid dynamics in particular the finite volume method, when you solve a fluid flow first you need to choose your domain of interest or the computational domain and in the commercial softwares, you need to create a geometry for this domain. And then as we already have the system of equations. So, if our flow is incompressible

and isothermal, then we just need to solve the mass conservation and momentum conservation equations.

If the flow involves heat transfer, then we also need to solve energy conservation equations. And the things become more complicated when flow is turbulent, but we will not go in the detail of turbulent flows; more so because as we discussed earlier in microfluidics flow is often laminar. So, in microfluidics application we are generally not concerned with turbulence flows.

The domain because it is always useful to have a smaller domain if possible; it is also good if you can decrease the dimension of the domain from 3 dimension to 2 dimension. So, if the things are not significant or if the velocity and velocity gradient in the third direction are not significant, then we can solve the problem in 2D in the Cartesian coordinate, it is in x and y coordinate and the third coordinate j g coordinate can be neglected v z is equal to 0, and del by del z for all the variables will be 0.

Similarly, in cylindrical coordinate system, where if the problem is axis symmetric; that means, if there is nothing happening along the azimuthal or angular direction, then v theta or velocity in the angular direction if it is 0, and the gradients in this direction is 0, then the problem can be solved as an axisymmetric problem and one need to solve only r and z equations. And then reduces the number of equations that need to be solved. So, our computational time and computational cost will be reduced.

So, that is about the computational domain. Now one can also take advantage of the symmetry of the problem, and can just solve the problem in half of the domain for example, a rectangular or square channel. Then one can solve the problem in one fourth of the domain with the symmetry boundary conditions on these 2 phases. So, once we have selected a domain, then we have domain boundaries and we need to define the appropriate boundary conditions on the domain boundaries.

For the wall generally, we have no slip boundary condition no slip means, that there is no slip between the solid wall and the fluid. So, that means, the velocity of the fluid adjacent to the wall is equal to the velocity of the wall. So, if wall is stationery then the fluid velocity is also 0. At the inlet we can define either a flow rate or a velocity profile or a pressure profile. Now velocity it can be uniform or it can be or there can be a profile.

When you define a uniform boundary condition, say for example, if this is flow between 2 parallel plates and if you define the uniform velocity at this, then there will be a ill posed boundary condition at these corners. Because the velocity will be 0 at the wall, but from the inlet the velocity is non-zero. So, you will see some problems, there the pressure take will take pressure will take unphysical values at those points, but generally this can be handled.

So, it is always a good idea to define a velocity profile which defines the velocity, or which has the velocity 0 at the walls. At the outlet one can have 0 gradient; which is generally known as outflow boundary condition, or constant pressure or a pressure profile at the outlet.

So, one can one has to define the domain, and identify the boundaries and give the appropriate boundary conditions at the domain.

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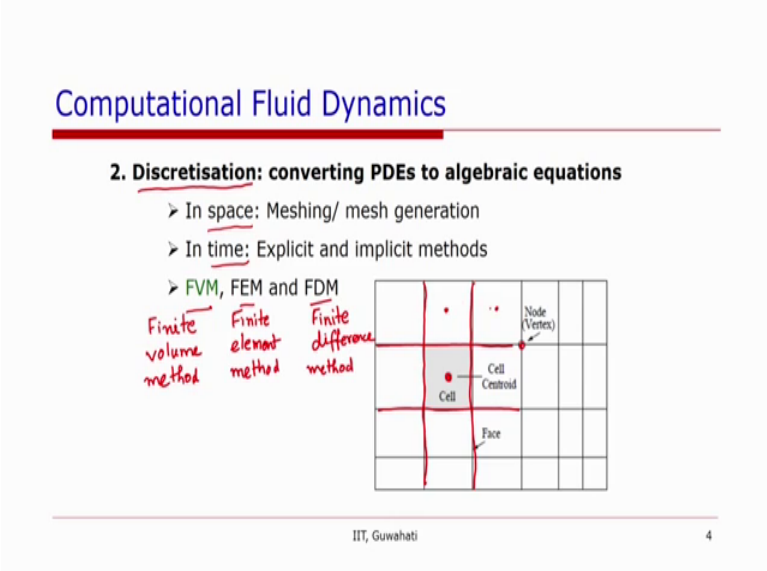

Once we have done that then we have formulated the problem; the equations are there and the domain in which we want to solve and the boundary conditions are there.

Now, we need to discretize it; so discretization is the process of converting the continuous partial differential equation into discrete algebraic equations. So, the process of converting a continuous equation into discrete algebraic equation is known as

discretization. So, when we do it for the terms which have derivatives in a space, for those we need to divide the domain or discretize the domain into a smaller parts.

Similarly, to solve in time, we need to have explicit or implicit time marching scheme; so we need to discretize in time. And there are number of techniques for discretization in a space; in computational flow dynamics 3 most popular techniques are finite volume method, finite element method and finite difference method. So, FVM is finite volume method, finite element method and finite difference method.

So, we are not going to discuss finite element and finite difference method we have been briefly, look at finite volume method. So, in the finite volume method; the entire computational domain, entire volume or entire area, depending on the problem is 2 dimensional or 3 dimensional is divided into smaller volumes or smaller cells. So, each the domain has been for example, here has been divided into different cells as you can see here; along these lines and the center of the cell, we call cell centroid and the intersection or these points are called nodes, and there are phases of the cells; this is not simple terminology.

So, in the continuous domain, or in when we have the partial differential equations, then we have the values or all points. Whereas in computational fluid dynamics we are discretizing and we get the values at the center of the cells.

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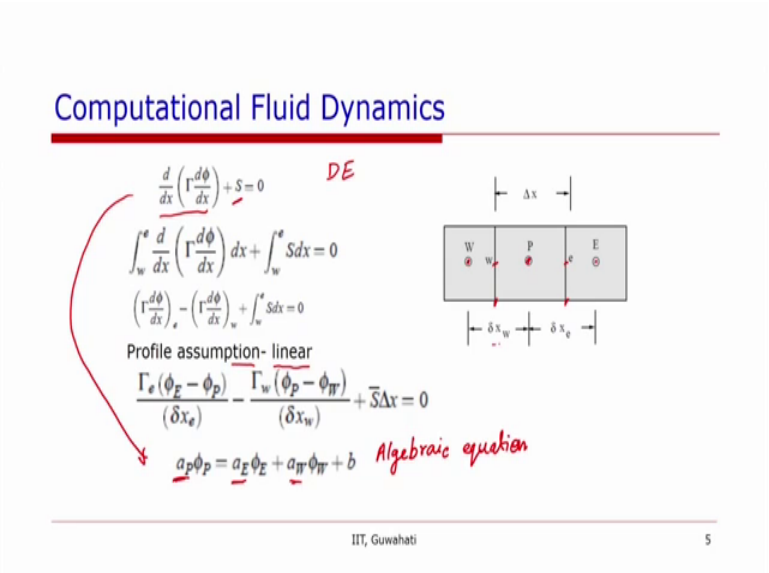

Apart from that so, what is done in finite volume method, what we have here is a simple diffusion equation with source term. So, this is the diffusion term, and this is source term and in finite volume let us say they are 3 adjacent cells for a one-dimensional problem. So, the length of the name of the cells or the cells enters are P which is point W a point on west of it and E a point east of it; the phases are being represented by small W and E small E for west and east sides respectively.

The distance between the points W and P and P and E is delta x; subscript W and delta x subscript E. Now let us integrate this equation d by dx and when we integrated and put the limits from west to east. So, this integration when we write then we can put it in this form after substituting the limits that gamma d phi by dx E minus gamma d phi by dx W plus integral W t x dx.

Now, when we integrate along these lines, then we need to have a assumption for the profile inside this, because what is the value of d phi by dx; so, we need to know that how the or we need to make an assumption that, what is the profile variation of phi in this at; the surface between W and P and between P and E. So, that can be used to find out d phi by dx at E and d phi by dx at W. So, if our domain is sufficiently small if our mass size; if our these elements are sufficiently small, then for any profile it can be approximated by a linear profile. So, that is what has been done here and phi d phi by dx is replaced by phi E minus phi P over delta x E similarly, for the other derivative and then it has been written.

So, when we collect these terms together and then right; so all the coefficients of phi P has been written into has a P and all the coefficient of phi E as a E all the coefficient of phi W has a W. And all the constant terms have been collected in b; so what we have been able to do that, we have been able to convert a differential equation to a algebraic equation, for one cell.

And the same exercise needs to be done for all the cells; the treatment will be different at the boundary nodes because the value at the boundaries will be known. So, we have to take that into account so that the boundary conditions can be used in the equations and then these number of equations are solved.

So, that more number of elements we have; the more number of equations we need to solve; that means, we need more and more computational time. That is why we are

always concerned about reducing the number of elements or reducing the computational load. But at the same time as I said that where the gradients are large, or where the curve is changing sharply, there we need to have more grid points to capture the accurate information.

So, the first process was that we discretize, or first process was we find out a computational domain, define the boundary conditions on this domain. Now the next step is discretized the equations. Once the equations have been discretized then solve these equations.

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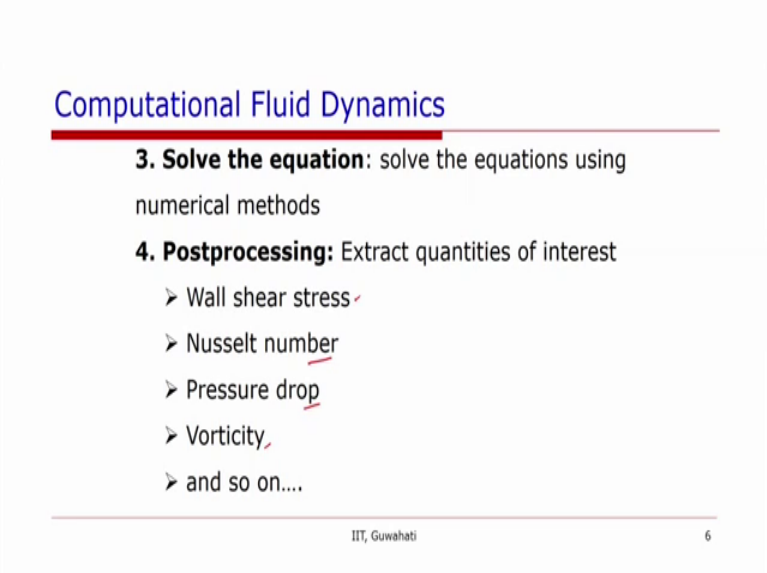

So, you have a number of algebraic equations, and then we need to use generally an iterative solver to solve these equations. And once we solve the equation, what we will get? We will get the values of the 3 velocity components, or the 2 velocity components depending on 2D or 3D problem and the pressure.

So, from that once we have solved the equations and got the values, then we can extract the quantities of our interest for example, wall shear stress if the heat transfer is there then maybe Nusselt number or pressure drop or vorticity or any other information that we can construct from this parameters that we have at our disposal. So, this is in very brief what the idea behind discretization is and how the partial differential equation is converted to algebraic equation, and what the term mass or an element or grid element mean.

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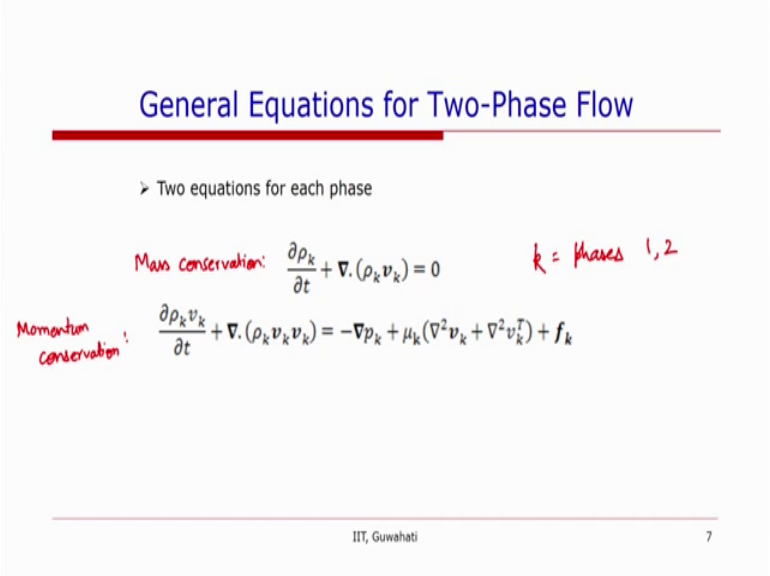

So now coming to 2 phase flow, as we discussed earlier that for a single-phase flow; we need to solve a mass and the momentum conservation equation for an incompressible and isothermal flow. Now, we have 2 phases then we need to consider one set of conservation equations for each phase. One for the phase 1 and one for phase 2; so, we have the 2 equations here, the mass conservation and momentum conservation equations k is phases. So, k represents different phase and it can be phase 1, phase 2; so, k is equal to 1 and k is equal to 2 and depending on we will have these terms.

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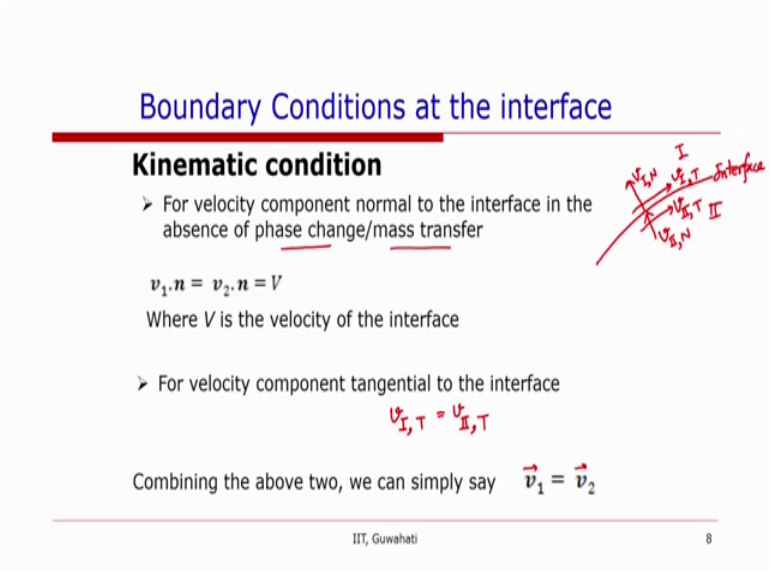

Now, at the interface because when we have 2 phase flow, they have the usual boundaries of the domain plus 1 boundary is the boundary between the 2 phases and this boundary would be moving; it is not a fixed boundary.

So, we also need to have the boundary conditions at the interface. So, as you might remember from you are if you have done a course on transport phenomena or then probably you would have studied. That for 2 phase; 2 fluid system, the boundary conditions, the kinematic boundary condition at the or the velocity boundary condition at the interfaces, that if there is no phase change or there is no mass transfer at the interface. So, if this is our interface between fluid I and fluid II.

And if then the fluid at this region is moving as a normal velocity component as v N; then this is v 1 N and this will be; sorry this is v 1 and this is v 2 and so, v 1 subscript N and v 2 subscript N. Now, if there is no phase change of mass transfer, then this interface will be pushed by a velocity v 2 and by this fluid, and then the same displacement will happen here.

So, the velocity at the interface or the normal component of velocity at the interface, or the velocity component normal to the interface; they will be equal in case of phase change or in case when there is no phase change, or there is no mass transfer. If there is mass transfer, because of phase change or otherwise then we need to take into account also the flow rate or the phase flow that there are flow that is happening from one phase to another; that we are not going to discuss here.

Similarly, the velocity on the tangential velocity component v 1 t in fluid 1 and v 2 t for fluid 2; they will also be equal. So, the tangential component are equal; the normal components are equal, and if you combine the 2, then you can say that velocity vector 1, and velocity vector 2 at the interface they are equal. So, velocity is continuous now; that means, the velocity is continuous at the interface, if there is no phase change or mass transfer in the fluid between the 2 phases.

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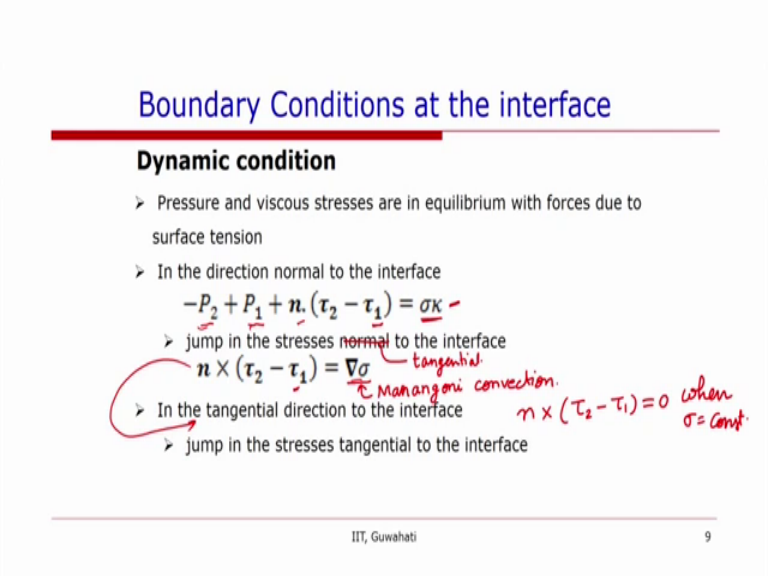

Now, the boundary condition for the stresses; so, let us look at the normal stress now. The normal stress, what we have pressure is also a normal stress. So, as you might remember from surface tension discussion, that the difference in pressure for the static condition P 1 and P 2; the difference between is equal to sigma kappa. So, the total jump in the extra tensor is a normal stress tensor. So, pressure as well as normal stresses, that might be there you could the flow that will be equal to sigma kappa.

Now, if there is Marangoni convection which is caused by the gradient of surface tension. So, this term is because of so, if there is a surface tension gradient, then we have jumped this is wrong this is tangential. So, this should have been here, and this should have been here anyway. So, jump in the stresses normal to the interface, is this where as in the tangential direction to the interface and crossed t 2 minus t 1 that is the tangential component of the stresses, that will be equal to del sigma; in case of there is no and this will be equal to; in case there is no surface tension gradient, when sigma is constant, then the tangential stress will be continuous in the interface, but there is a jump in the normal a stress.

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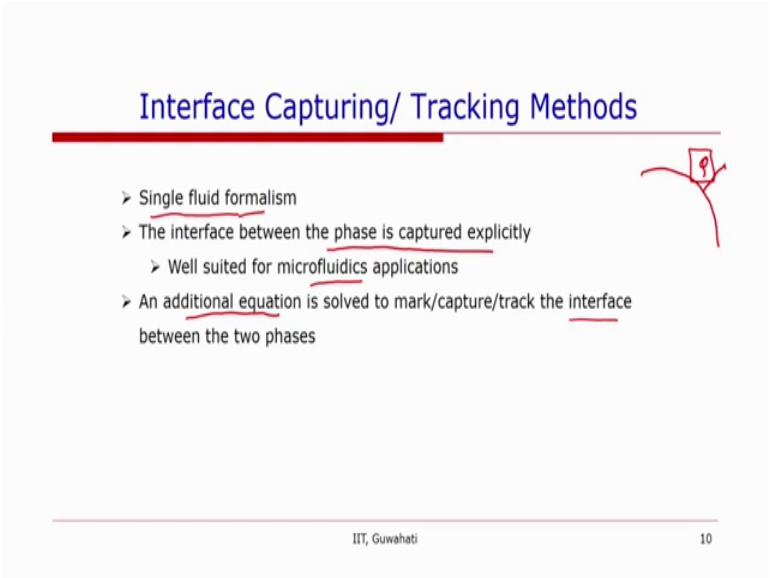

So, for the 2 phase flows; we have written down the equations, and we have understood the boundary conditions. Now there can be number of different approaches to model multiphase flows. You might have heard about Eulerian multiphase flow modeling method, or Euler langregian multiphase flow modeling method, or you might have also heard about the volume of fluid method, level set method or in general the term which is called interface capturing method which are used to model multiphase flow.

So, the question comes which approach one should take to model multiphase flow method not a methods. Say in general for the industrial applications for conventional multiphase flows; the number of bubbles, the number of droplets that are there in a system. For example, consider a bubble column which is a column of liquid in which the gas bubbles are introduced and the number of bubbles are millions. So, if the one to capture the bubbles in this column, then we need to have the interface; if you want to capture the interface at each and every bubble, then we need to have very refined mass.

So, in general in such cases the equations are averaged, and the exchanged between the 2 phases, momentum exchange and if there is a heat transfer or mass transfer exchange. That is modeled by closure terms; so, that the computational time and computational cost is reduced and a still one can find useful information about the flow. However, when it comes to flow in micro channels, then the number of bubbles are limited.

Flow is often laminar and it is quite regular; so, in such cases we also see that the interface is quite large, or the interface is quite big. So, one there is a motive or there is a motivation to capture the interface and capture the information accurately; rather than having a closer model which will come from either from the experiments or from some heuristic or empirical models.

So, generally for most of the cases in micro fluidics one do not need to have one do not huge of Euler; Euler method which are generally based on the averaging of the equations. Rather one usage interface capturing or interface tracking methods; so, let us look at what those interface tracking methods are. In this case, a single fluid formalism is applied; that means, only one set of conservation equations, even though we have 2 fluids, or more than 2 fluids, then let us talk about only 2 phase flows.

So, even though we have 2 fluids, only one set of conservation equations are solved, and the interface between the 2 phases is captured explicitly. So, such things or such case will be well suited for microfluidic applications when we have one droplet going in the channel or few bubbles going in the channel, and we can capture the flow behavior by stream lines and the bubble velocity, the droplet velocity, the heat transfer and so on.

So, when we have 2 fluids being modeled by a single sort of equation, then we also will need something by which we can identify the 2 phases. And we can distinguish between the 2 phases; for that one additional equation is solved or one additional for the advection of the interface, and this particular feature distinguishes different methods which are there to model 2 phase flows. For example, in the volume of fluid method, the volume of fluid that is present in a cell is used as a marker function and that is how one identifies the interface.

In level set method, the interface is a level set function is solved or the level set function is equation for the advection of the level set function is used. So, what is level set? That means this is the interface, then distance from the interface is called level search function.

So, that means that the function when phi is equal to 0 that represents the interface. So, del phi; so the equation is solved for the advection of phi and the phi is equal to 0 represents the interface. For solving multiphase flows, one uses generally interface capturing methods have been used, there are number of other methods, but we are going

to describe the general approach and the leaders are referred or the students are referred to look at another move scores or look at further literature to know more about these models.

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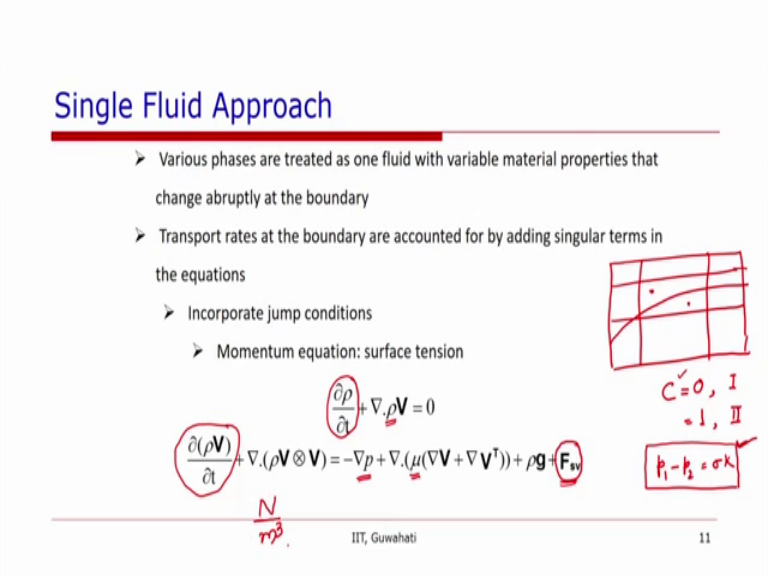

So, in the single fluid approach, we treat that all the phases are one material. Now if you look at these equations, in this we have 2 properties. One is density, and another is viscosity of the 2 fluids. So, one need to identify, when we have an interface and it this interface is to be captured than in such case, we will have at any point in a space, except at the interface; one will have that the fluid is either fluid 1 or fluid 2.

So, if it is in fluid 1, then we use rho 1, if it is fluid 2, then we use rho 2; similarly, for mu. So, the properties are variable, and we have to define it in such a manner, that if we have a marker function C, which tells let us say if it is 0, in fluid 1 and it can be 1 in fluid 2. So, once we have identified based on the marker function, that in which fluid we are; we can use the properties of those fluids in these equations. So, basically by having variable properties we are solving 2 equations. Now comes the interface the boundary conditions at the interface.

So, the boundary conditions that we will use at the interface are if you remember the boundary conditions that we discussed that the interface, we need to have a velocity continuity. Because at the interface; in the absence of evaporation and mass transfer, the normal components in the 2 fluids are equal tangential components in the 2 fluids are

equal; so, that means, velocity is continuous. In any way, in any case, the velocity for our system of equation is continuous. So, the velocity continuity is inherently built in this system of equations.

The next part is the dynamic boundary conditions at the interface. The first one is the tangential stresses; so, if there is no Marangoni stress, then the tangential stress is continuous which is inherently built in the system of equations, the stresses are going to be continuous; so, fine. The other boundary condition which we had is; the normal stresses or let us say P 1 minus P 2 is equal to sigma kappa; which is becoming because of the surface tension. So, and that will also take into account that the surface tension in the 2 fluids are different.

So, we have a model or a term which can take account take into account this jump in boundary condition or in the normal stress or tracer at the interface. So, to take that into account this new term has been added which we call as F SV and we will discuss this in later slides. So, in summary what we have looked here is that in the single fluid approach, we still solve the navier stokes equation, only for only one fluid. Now for this one fluid we have the density and viscosity; these are the 2 properties of the fluids.

Now, the question comes which fluid properties; so, we have a marker function, and we need to know with this marker function; if we know let us say we know the values of the marker function in each grid, then we will be able to define that what is the value of rho, and what is the value of mu at any cell. The cells that have interface in them, in those cells we will have the viscosity and density as the average volume fraction weighted average of the properties of the 2 fluids.

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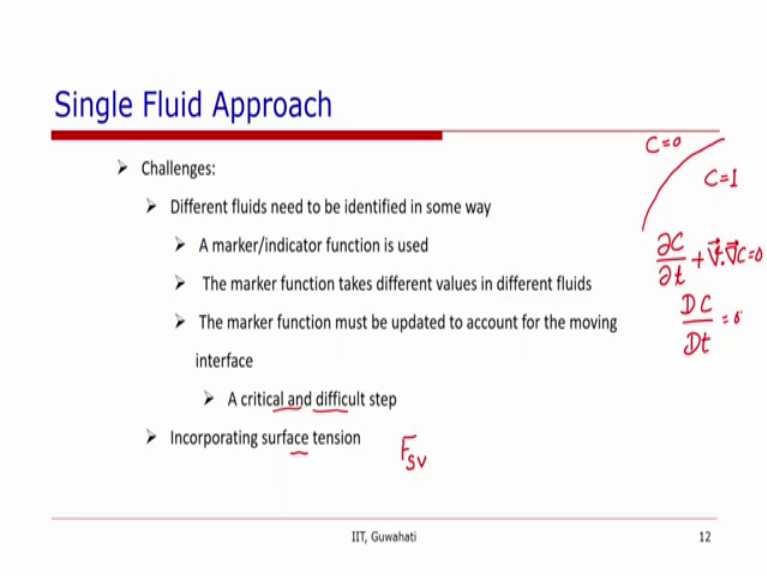

Now, there are a number of challenges, or number of issues that we need to address to use a single fluid approach to model 2 phase flow. The first thing is that as we were talking about that when we have a 2-phase system, and we will have a marker function, that C is equal to 0 in one phase and C is equal to 1 in another phase. So, we need to have a marker function; so, we need to solve a equation advection equation in terms of del C by del t plus v dot; the velocity vector dot del C is equal to 0.

So, or we can say that the material derivative of this is equal to 0 for this marker function. So, the marker function takes different values in different fluids. And each time the marker function must be updated to account for the moving interface, when the interface is moving. So, this is a critical and difficulty step in some cases; we also need to take into account as we just discussed that the surface tension jump should be taken into account and how this the term we had F SV in this system of equations how that can be modeled.

So, one need to take into account that the terms that we have in the navier stokes equation, if we go back to these equations every term is say for example, in the momentum equation, we have force per unit volume. The unit for each term in the momentum equation; if you look at the easiest to look at is rho g. So, if this term is in terms of force per unit volume or for example, pressure is force per meter square and it is damage per meter; so Newton per meter cube or forced per unit volume.

So, this is true for a body force the terms are for the different body forces. Now if you look at the surface tension; surface tension is a surface force which acts only at the interface. So, this is basically or it is not exactly a force it is a jump in the pressure or normal stress at the interphase. So, how do we incorporate this in is equation which has; which all the terms are body forces? Or how do we convert this into a body force or a volume force?

So, this is done using Green Gauss theorem and the surface integral is turned is converted into a volume integral using Green Gauss theorem, and then surface tension force is used as a body force in the momentum conservation equation as a source term.

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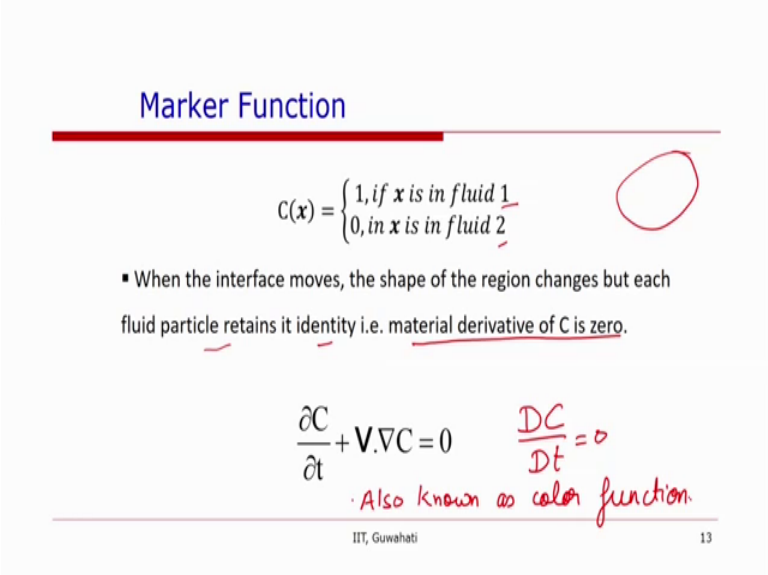

So, let us look at the marker function, marker function is that it has one value one in one fluid and 0 in another fluid. And when this interface moves; so, when the interface moves, the shape of the region changes, but each fluid particle has it is identity so; that means, this material derivative is 0. So, that is why we have del C over del t plus v dot del C or DC by DT is equal to 0.

So, that is how one more equation; so, we had 2 conservation equations mass conservation, momentum conservation plus 1 advection equation for the color function or the marker function. This marker function also known as color function; so, we can write here that it is also known as color function.

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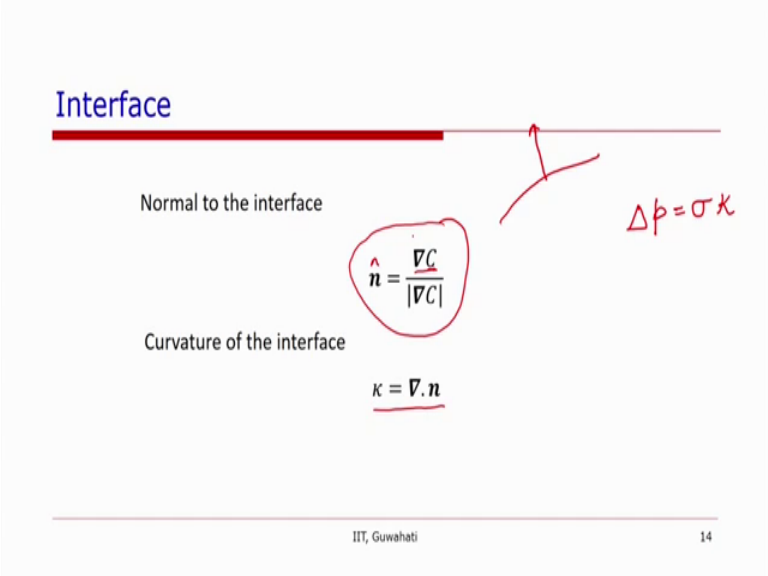

At the interface, when we want to implement something or when we want to implement the surface tension force, then we need the curvature. If you remember the pressure jump at the interface or Laplace spacer is defined as sigma kappa; where kappa is curvature of the interface.

So, we need to identify the curvature of the interface. And this information can also be obtained from the color function or from the marker function. So, the unit normal to the interface; that means, the vector normal to the interface at any our self it can be obtained by del C over the magnitude of del C vector or the gradient of color pencil vector. Once we have obtained the normal to the interface, the curvature is obtained by del dot n; if from the relationship the curvature is del dot n. So, from this we can calculate the curvature.

So, lot of implementations of a volume of fluid method, the inaccuracies or the problems that occur; they occur because of the inaccurate definition of or the inaccurate implementation of n.

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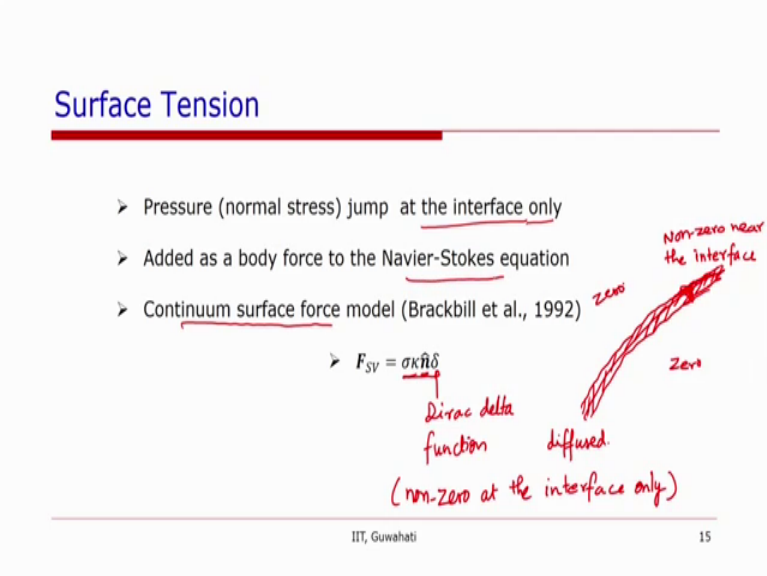

Having clarified that marker function or that we need to solve one equation for the marker function, and how do we find the curvature of the interface. Let us look at how we can include the surface tension.

So, the surface tension jump or the pressure jump at the interface is non zero at the interface only. So, at the interface we will define function which is 0 everywhere else, and non zero at the interface. So, if we have we have plotting it an on a scale; so, the value of so, the value of this force is non-zero near the interface, 0 everywhere else.

And in these methods, one need to appreciate the fact that the interface in reality is of almost 0 thickness; however, the interface is fairly thick in several other cases. The interface is quite thick in real (Refer Time: 45:14) interface is thin, but in the computational methods it is at least one cell or one element thick because it is being discretized. So, the interface is what is called the interface is diffused.

So, the surface tension force is also diffused over the area, or it is distributed over the area in which the color function is between 0 and 1. This surfaces tension force is implemented only at the interface for the sigma kappa n gives the direction of the force. And del is dirac delta function, which is non zero at the interface only and this model is known as continuum surface force models of the surface force is converted into a continuum forced and included in the system of equations of the navier stokes equation as a body force.

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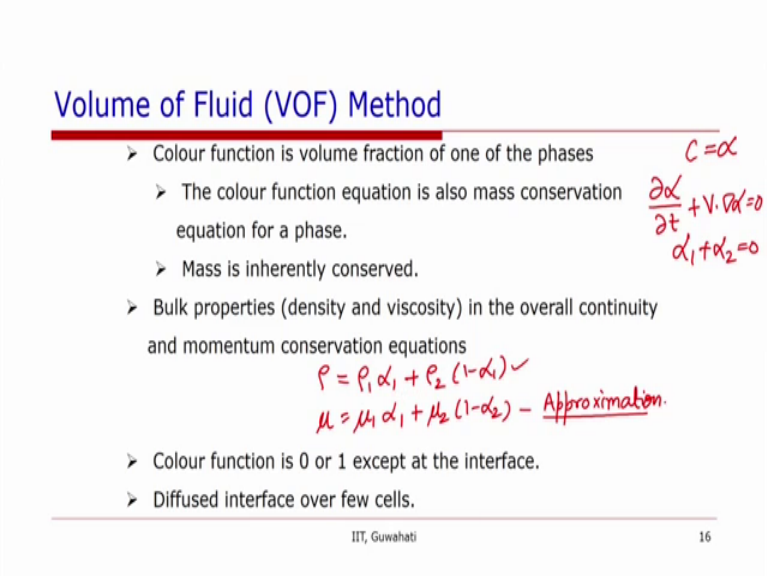

So, what we have described is the general a structure of any single fluid for a formulation or single fluid approach to model 2 phase flow. In volume of fluid method, this color function or C is equal to alpha, where alpha is volume fraction of one of the phases. So, the equation becomes del alpha over del t plus V dot del alpha is equal to 0, and if you look at this equation what we get is the mass conservation of amount of edges. And alpha 1 plus alpha 2 is equal to 0; so, basically what this gives the conservation of mass for each phase.

So, the mass of each phase is inherently conserved which is not the case for other methods. And in this case once we have obtained alpha, the rho is equal to rho 1, alpha 1 plus rho 2; 1 minus alpha 1. Similarly mu is equal to mu 1 alpha 1 plus mu 2 1 minus alpha 2; while this is accurate and it can be proved, this is just an approximation. But generally, works fine for most of the cases. So, you can see that accepted the interface this rho is equal to rho 1, we have alpha is equal to alpha 1, and rho is equal to where alpha 1 is equal to 1 and rho is equal to rho 2 and alpha 1 is equal to 0; this is about the interface capturing methods.

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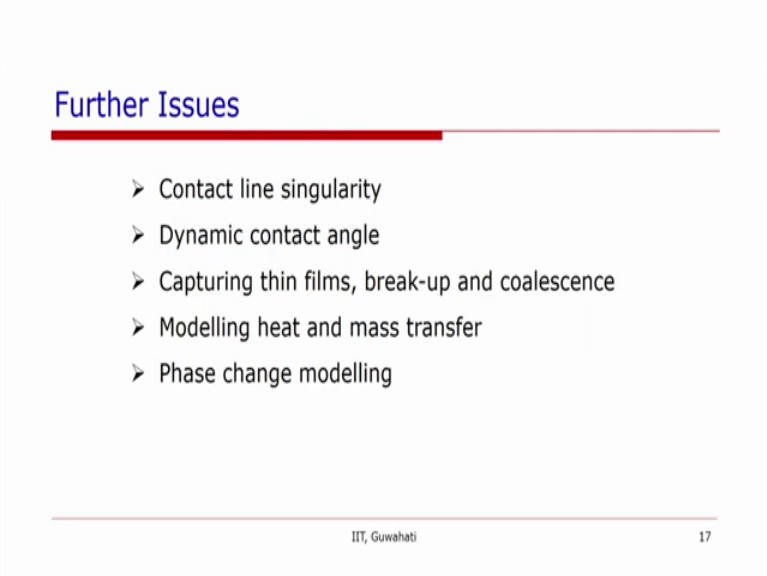

Now, there are number of other issues other problems that one need to look at when modeling to phase flows. For example, the contact line or 3-page contact line plays an important role in number of micro predict flows. So, one need to take into account that how do we model the contact line singularity near the interface. Because the contact lineage move in what is the contact angle and the contact angle it is a dynamic contact angle; so, one need to have a model for dynamic contact angle.

Sometimes the films are very thin in micro predict flows. So, one need to have the mass very, very refined so that the thin film flows can be captured. Similarly, during coalescence or breakup of the bubbles; the films that form between the 2 phases are very thin. Sometimes of the order of few nanometers , and one cannot have over cannot afford to have such small very such a small mass, because that will require over the length scale changes about 5 to 6 order of magnitude.

So, how one can model such thin films or the thin films that forms during breakup and coalescence. Heat and mass transfer especially capturing the boundary layers near the interface accurately when condensation or interface mass transfer or evaporation happens and similarly, is of for the phase change modeling.

So, in summary in today's lecture, we have first looked at specially for those who have not been introduced to computational fluid dynamics. First, we have looked at the basics of computational fluid dynamics, and then one is encouraged to read through books for;

if they want to study the computational flow in computational fluid dynamics of the book by pattern curve numerical fluid flow and heat transfer.

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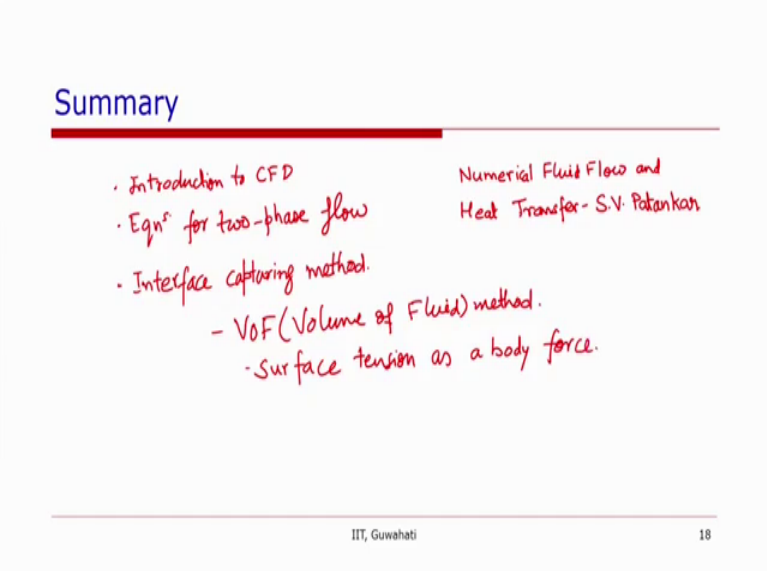

My S. V Patankar can be a good starting point to understand the basics of combinational flow dynamics especially the finite volume method.

And then so, we have looked at the basics of or very briefly what computational fluid dynamics is. And then we have looked at the governing equations for general multiphase flows or general 2 phase flows and then what are the boundary conditions at the interface for these flows. Then we have come to the interface capturing method; so, first we introduced CFD. CFD, and then equations for 2 phase flow and then we have looked at interface capturing method, specially the VOF or volume of fluid method, in which the surface tension; how it is used as a body force in the navier stokes equation. So, that is all.

Thank you.