Introduction to CFD
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Lecture - 51
Basics of Interface Capturing Methods for Applications in Multiphase Flow (continued)

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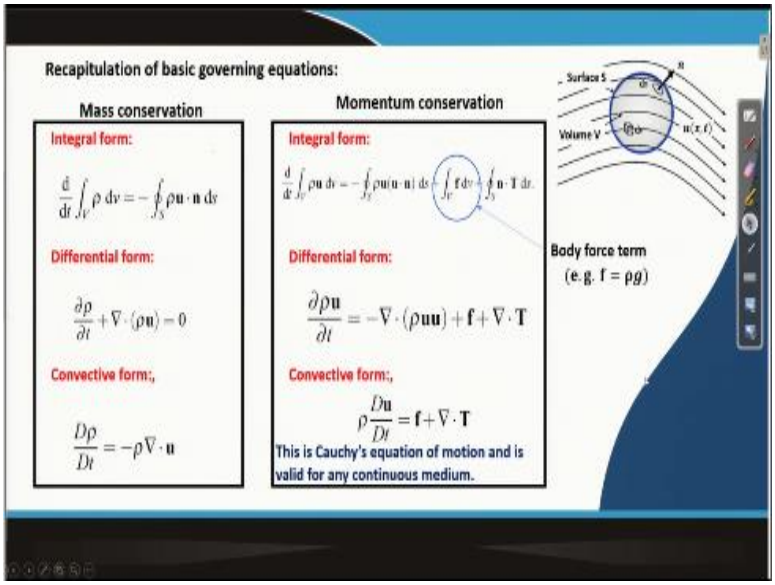

So, we continue our discussion on interface capturing techniques for multi phase flows. So, in the previous lecture, you recall that we were discussing about the basic governing equations, and we had discussed about both mass and momentum conservation at some length.

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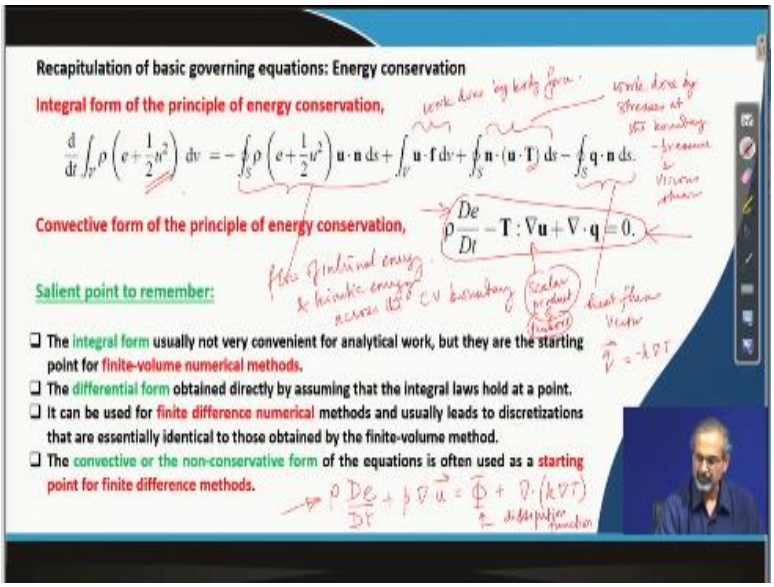

And now, we will look into the next conservation equation that is incidentally the energy conservation. So, in energy conservation equation, of course, we look at the rate of change of internal energy and kinetic energy. And that is the term which figures on the left hand side of the equation and on the right hand side, the first term is the flow of internal and kinetic energy across the boundary. So, that is this first term.

So, this is flow of internal energy and kinetic energy across the control volume boundary. That is the first term then comes the body force, which does work, so, we can write it as work done by body force and the subsequent term is the surface stress term. So, work done by stresses at the boundary, this would include pressure and viscous shear. So, you remember that the stress tensor that we had expanded in the previous lecture included pressure terms as well as viscous terms.

And then the final term, it is the heat flux vector q, which is dotted with the normal vector. And if you look at the Fourrier law, then this can be of course, indicated in terms of the product of thermal conductivity and the gradient of temperature with a negative sign indicating the direction of heat flow. And this equation can be of course, further simplified by making use of the momentum equation and dotting it with velocities.

So that we have an equation for mechanical energy, which figures over here and then if we subtract that equation, then we will end up with an equation in terms of the internal energy alone and then you can apply the definition of substantial derivative. So, that you have a form of this kind and in this equation, you see a scalar product of 2 tensors. And further this equation can be represented in another form where you can write it like this.

And in order to write it like this, you make the assumption that you are applying the previous equation to a Newtonian fluid. You are neglecting radiative heat transfer. And then the energy equation will boil down to a form like this which includes this capital phi which is called as the dissipation function.

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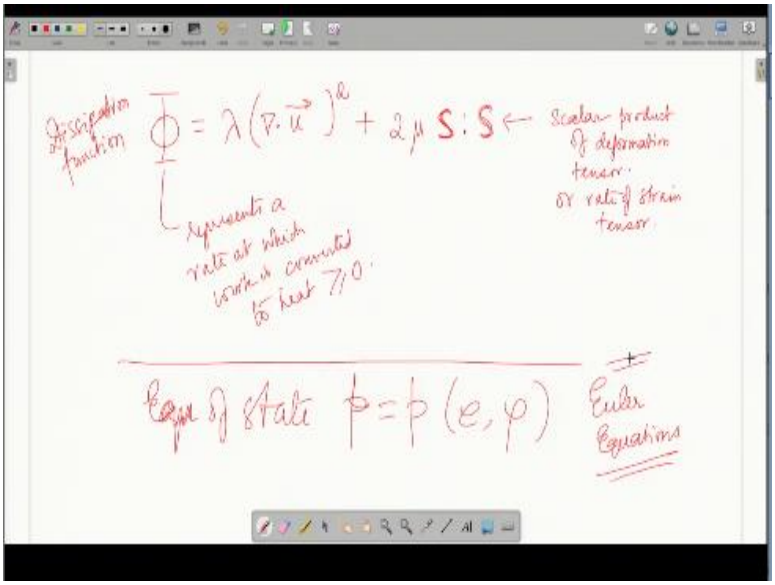

And if we just try to recall, this dissipation function capital phi is essentially lambda times divergence u whole square plus 2 Mu plus scalar product of S. We recall that S is the deformation tensor. So, you can also find it mentioned as rate of strain tensor in books and you always need to remember that this dissipation function represents a rate, it represents a rate at which work is converted to heat.

And of course, it always is greater than equal to 0. In addition to these conservation equations, we will also require an equation of state to solve these equations, equation of state and we can write it in a functional form like this for example, p is a function of each row. You remember that we had in such a equation of statement discussion about Euler equations in the previous week.

So, this more or less sums up the brief recapitulation of the governing conservation equations of mass momentum energy and then, when it comes to numerical solution, we have to recall that you know, you can have them in integral form, which is often the form which will be preferred for finite volume methods or differential form, which is when you take the integral laws and apply them at a point, you come up with the differential forms.

And those forms are more amenable for finite difference methods. And you could either have conservative or non conservative forms of these equations. And accordingly the formulations will be decided according to what form of equations you are using.

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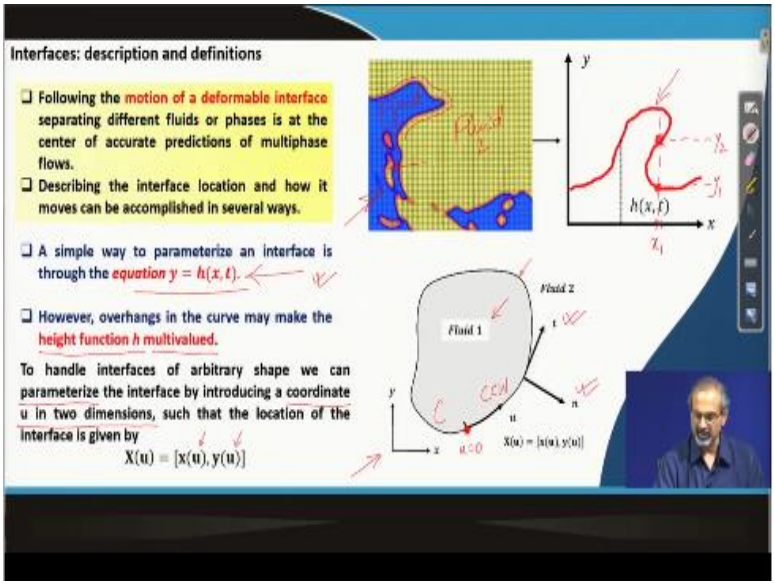

Now, a little bit on what we mean by interfaces and how do we describe them. So, we have a few points here. So, we are following the motion of deformable interface which is separating the different fluids or phases and we have to model it accurately and that is at the heart of correct or good quality predictions of multiplayers flows. And we have to have a suitable method by which we describe the interface location.

And also a method by which we define its movement, because, these interfaces are always in general unsteady, they are going to change with time. For example, if you look at this figure here, you can make out that there is a fluid here in the blue region if we call it as fluid 1, there is another fluid in region two for example, and then they are interacting with each other.

It is almost like looking at a small portion of a breaking wave, where you can see that some portions of fluid 2 has even got into the fluid 1 region and there are almost continuous interfaces in certain regions. And then there are discrete interfaces and certain others and so on. And a simple way of parameterizing the interface could be an equation of this kind for example, in a two dimensional situation.

So, in a two dimensional x y plane, if you have a fluid region 1 defined like this, with an interface shared with fluid region two, then one way of defining it could be through an equation y equal to h, h being a function of x and t. But the fallacy of this approach would be that if you have interfaces which comprised of concave and convex regions, then very often you may come up with multivalued form of this equation y.

Because as you can understand at this x, let us call it x 1 you will have 2 values of y, so, you can call them as y 1 and y 2. So, at x 1 you do not have a unique value of y and therefore, this kind of formulation will have difficulty in tackling such an interface. So, if we call this h as a height function then height function becomes multivalued. But, if you have a parametric approach, you can handle the interface better because in that case, let us say the interface is handled by introducing a coordinate u in two dimensions.

Such that any location on the interface becomes a function of u, u is like a running coordinate which is moving along the periphery of the curve. Let us say the curve is C. So, you have a starting point defined where u is equal to 0 from that point you are trying to move counterclockwise along the periphery of the curve and trying to come back to that original point and in that case, you will not have the problem which the height function had faced.

And then based on this functional description, you can of course, define the normal and tangent vectors for example, by taking derivatives of that capital X function which is a function of u essentially. So, this is the manner in which one can go about doing the calculations with a parametric approach. Of course, the parametric approach can become more involved when you go into three dimensional space.

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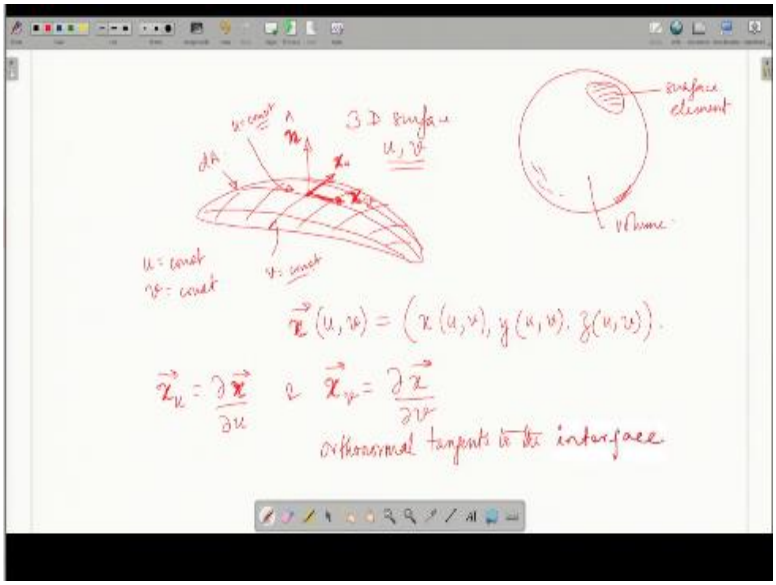

For example, if we have a situation like this, that you have a surface say a spherical surface and then on that surface you have a small region defined and then we are trying to find out the geometrical aspects of that small region. So, we call that as a small surface element for

example, and this is the bigger volume. So, in that case, let us see how the geometry can be defined.

So, the geometric aspects of that small surface element can be kind of sketched like this, if we look at that surface element more closely. We may find that there are lines which can be defined to wrap up this this surface, but you will need at least you will need precisely two families of those lines to cover up that surface in 3D. So, if it is a three dimensional surface, you need essentially a parameterization through 2 variables u and v of the 3D surface.

So, if you have that you will have u equal to constant lines and v equal to constant lines which wrap up that surface. And if you look at any point where these interact, then of course, based on the definition of that surface, you can always calculate the gradient of the function and define the normal the unit normal vector of this small elemental area dA at that point, where this line is say some v equal to constant line.

And the other line which comes in from the other direction is the u equal to constant line and these constants will vary as you move from one line to the other of the respective families. Now, with the normal define there, you can have definition of two tangents there, x u and x v. And then in general x is a function of u v where this vector x is represented as and remember that these are vectors.

How do we define the vectors x u and x v? So, that is del x del u and x v is equal to del x del v that is how we define them and they are both tangent to the interface. So, they are the orthonormal tangents to the interface.

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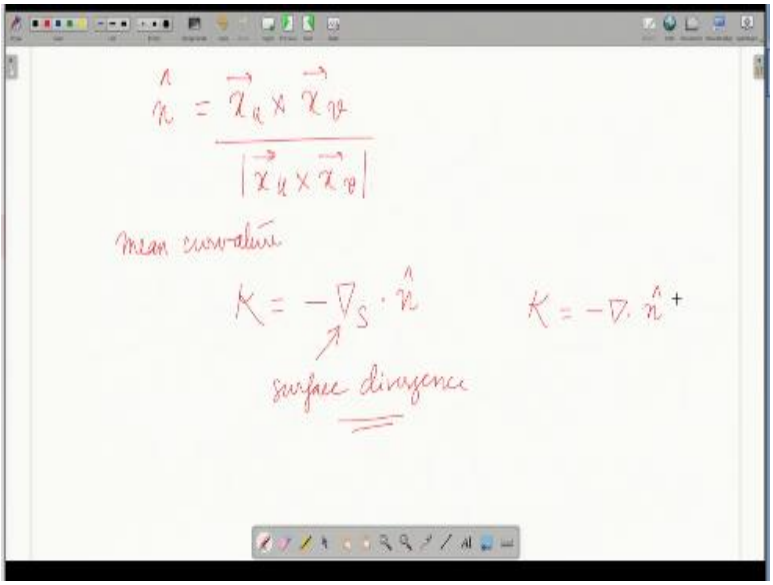

Now, you can show that x u and x v satisfy this property that if you take a cross product, they will give you the normal vector. And then additionally, if you are interested in finding the mean curvature of the surface and that point the curvature Kappa can be indicated by divergence of the normal vector and this Nabla S denotes the surface. The Nabla S dot indicates the surface divergence that means, as it applies to that surface.

So, these are some of the concepts which we will see even in the remaining slides later. And Kappa in general can be also defined as divergence of n as you move away from the surface in the normal direction.

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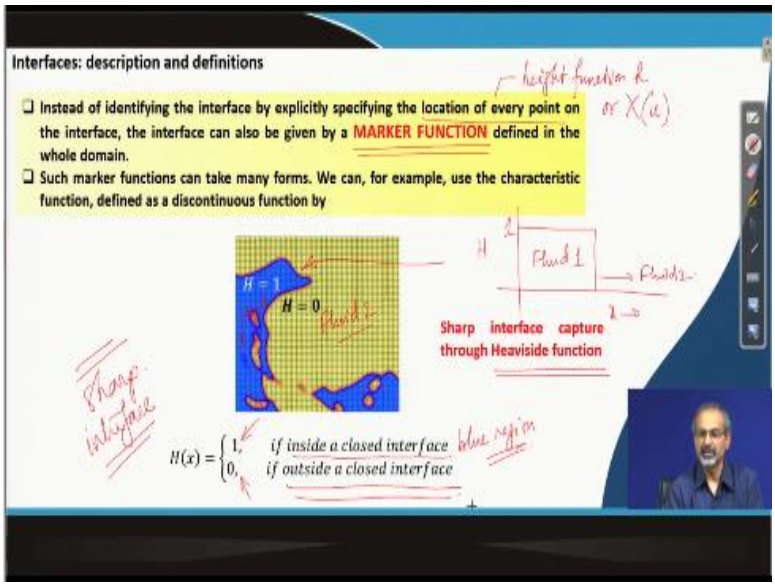

So, these concepts will come in handy, going over to the concept of Marker function. So, if you are capturing the sharp interface, then there would be a jump in the value of a property

and in this case, we will say that we define the value of one of the phases through a heaviside function which is nothing but a step function which attains a value of 1 inside the closed interface that means in the blue region and it will attain a value of 0 otherwise.

So, it is outside of the closed interface. So, if that is the case, we can just look at the bullet points instead of identifying the interface by explicitly specifying the location of every point like we were doing to the height function that is h or to the parametrization of the function x which is essentially a function of the running coordinate u. The interface can also be defined through Marker function.

That means we are as done marking the different phases with some kind of functional value of this heaviside function then, such Marker functions can take many forms. Okay. So, in this mathematical sense, it is what is called as a sharp interface that means, there is a step jump in the value of h as we move from the face. If I call this fluid 1, then as I move from fluid 1 to fluid 2, there will be a step jump in the value of h.

That means if I try to look at it in a cross sectional sense, it will look like this. So, if a certain cross section of the two phases look like this that fluid 2 lies here and fluid 2 lies beyond this. Then the value of h as a function of x will then be either 1 when it is fluid 1 or 0 when it is fluid 2. So, it is a step jump or a sharp interface. Now, it may so happen that when we compute these phases, how they are emerging with time.

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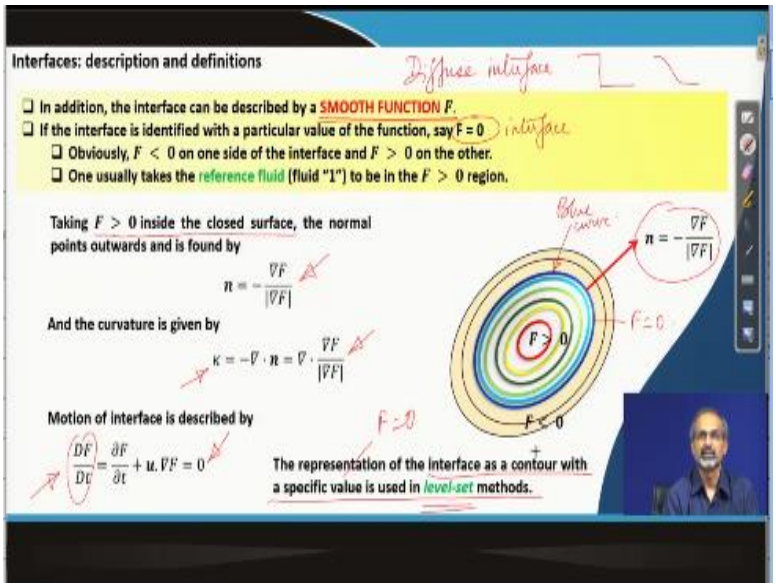

We may not be able to always handle them as very sharp interfaces, but rather through slightly diffused interface. That means there will be changes in the properties, but it will happen through slightly larger landscape in which case, we would call such an interface as a diffuse interface. That means instead of a step change, let us say, it is some moderate change.

So, like we talked about heaviside function being used as a step function, which gives the tool to handle an interface as a sharp interface, we can also have smooth functions. And we will introduce a smooth function F such that if the interface is identified with a particular value of the function say F = 0 then it will be less than 0 on one side and greater than 0 on the other. That means F = 0 is the boundary or the interface.

And F changes to a negative value in one region of or one phase and becomes positive in another region or another phase. So, how can I come up with a definition of F? Let us see that in this case, how we go about it is we first take F greater than 0 inside the closed surface and the normal then points outside and it is found by gradient of **(()) (21:55)** F by the modulus of F with a negative sign.

So, that is the unit normal pointing out of F. So, F is greater than 0 inside this blue curve which is essentially the boundary and ideally we should be having F = 0 at the boundary. The curvature as we discussed earlier can be found from minus divergence of n. So, it is expressed like this and the motion of the interface is then described by the material derivative of F.

Now, what it means is that F as it moves through the fluid domain would carry along with it the information about F. that means a fluid particle no matter where it moves into the flow field does not lose the value of F that it is carrying along with it and that is what is called as the material derivative. And therefore, motion of the interface no matter where it goes will always be defined by the the substantial derivative of F = 0.

Now, this kind of representation for the interface as a contour with a specific value in this case it is F = 0 is used in one category of methods which are used for interface tracking which has cordless the level-set methods.

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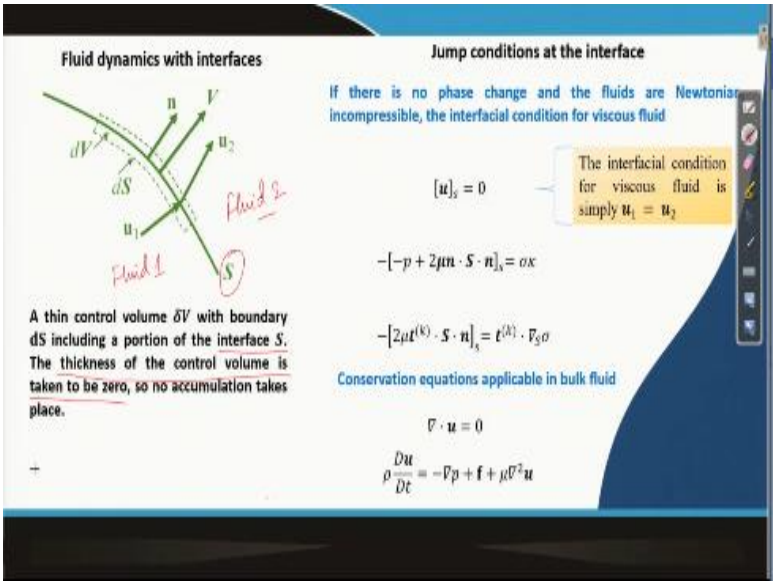

Now, getting a little deeper into the fluid dynamics with the interfaces, we have an interface here represented up or other a portion of an interface represented in a kind of an elemental manner. So, here the interface is actually defined by this S and as you can understand that this may be part of the boundary of one of the phases. So, on one side of the interface you may have a certain fluid say fluid 1.

And another side you may have another fluid say fluid 2 and then you have a thin control volume, this delta V with boundary dS which is surrounding this portion of the interface and we assume that the thickness of the control volume is limit, it limits to 0. And therefore, if you limit it to 0 then there can be no accumulation handled by this interface. So, no property can actually end up accumulating at this interface, because of the thickness limiting to 0.

Now, if that is the case, then you can very well show that in terms of say, mass conservation, let us see how it works out.

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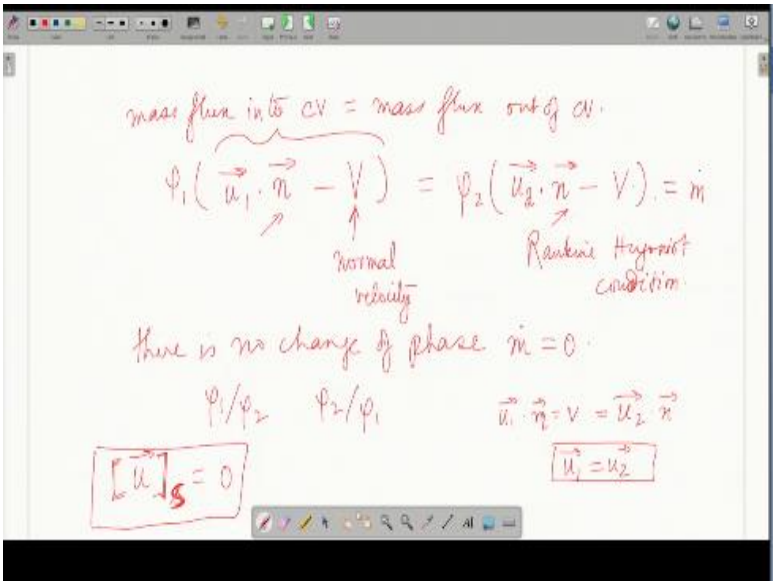

So, if you look at the diagram, you can show that mass flux into the control volume will be equal to mass flux out of control volume and then you have the fluid velocity u 1 on one side that is in the fluid region 1, which if **(()) (25:18)** dot with the unit normal vector will give you the normal component of the fluid velocity on the region 1 and because the interface is moving with some velocity V where this is already given as a normal velocity.

Then this is this expression gives you the net velocity at the interface in the normal direction. Alright. So, this is the velocity on region 1 and then accordingly you can find it out for region 2 like this. And then if densities are row 1 and row 2 on the two sides, you can multiply them with this net normal velocity and they should give you the mass flux across this control volume.

This is nothing but the Rankine Hugoniot condition which we have learned when we talked about shock waves in courses on compressible flow and we said that there is no mass accumulation, but the other point that we need to keep in mind is that if you assume that there is no change of phase at this interface, then further m dot should be equal to 0. Now, if we are handling incompressible fluids, then these densities row 1 and row 2can be different for different fluids.

So, for arbitrary density ratios, which will be produced either in the form of row 1 by row 2 or row 2 by row 1 irrespective of whatever values they have, you have to satisfy this equality and then that is possible only if these bracketed terms are individually 0 and that means you

have u 1 dot n = V which is again equal to u 2 dot n. Only then it can be possible and you can then very easily show that u 1 should be equal to u 2 in that case. Only then it is possible.

Now, you can represent this information in the form of a more compact nomenclature, which is the nomenclature of jump condition. So, the jump in u which is expressed as a square bracket across this surface S is equal to 0. So, this is the concept of mass conservation across this interface. And you may recall that this was the nomenclature used in the previous case. Now, similarly, we can do more on the other conditions.

So, we already indicated this as a jump condition equal to 0. That means the interfacial condition for viscous fluid is simply u 1 = u 2. The other two conditions are essentially coming from the surface tension.

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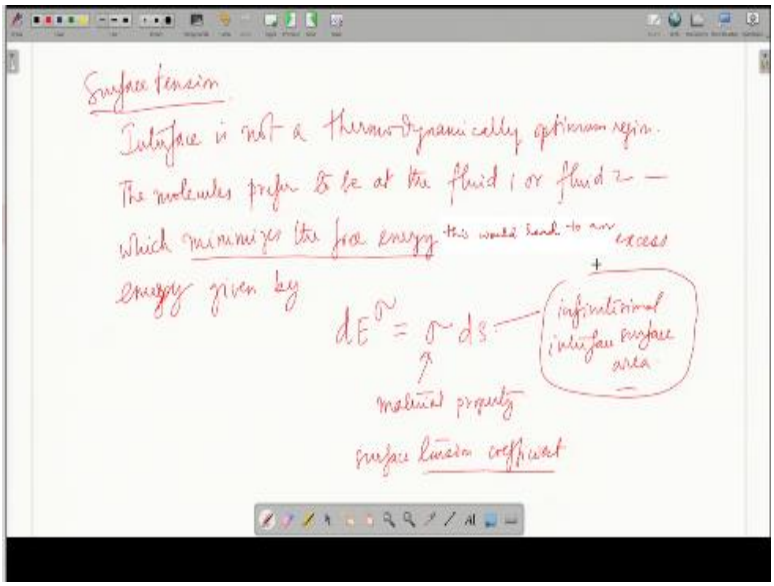

So, if you look at the surface tension part of the story, then we just note down a little on surface tension. So, as we know that surface tension arises because of the interface is not a thermodynamically optimum region. So, interface is not a thermodynamically optimum region. Why do we call it like that? It is because the molecules which are on two sides of the interface.

They prefer to be at fluid 1 or fluid 2, the choice based on which minimizes the free energy. Now, this would lead to excess energy, because of the non optimum condition which is given by dE sigma = sigma dS, where sigma is a material property. And it is usually referred to as

surface tension efficient. And dS is nothing but in finitesimal interface surface area. So, this is how the free energy minimization works at the interface.

And this is how it links with the surface tension coefficient and the interface surface area. So, we will discuss more on this aspect in the next lecture, and we will try to explain a little further on these two equations and move on. Thank you.