Microfluidics
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Lecture - 03
Micro-Scale Fluid Mechanics

So today we will look at micro-scale fluid mechanics. So before we talk about micro-scale fluid mechanics let us try to understand what a fluid is. A fluid is a substance that deforms continuously under the action of shear stress.

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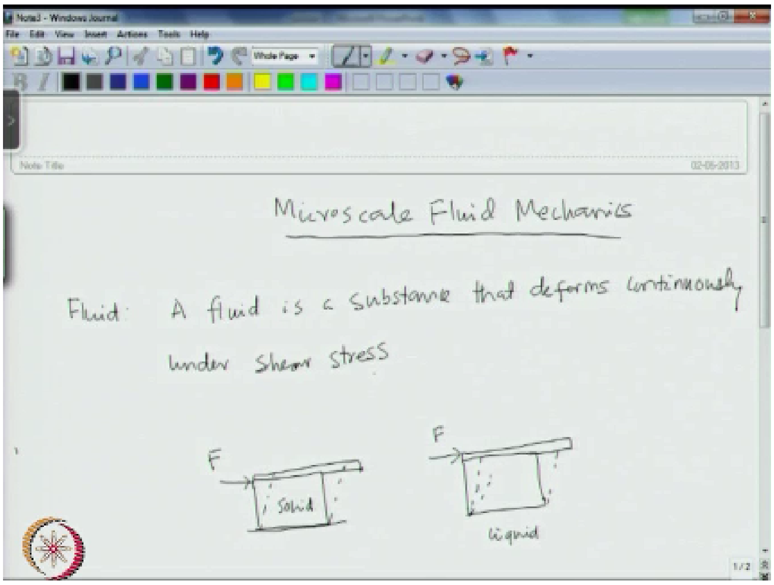

Micro-scale fluid mechanics so first try to understand what is a fluid? A fluid is a substance that deforms continuously under shear stress. So a fluid is a substance that deforms continuously under the action of the shear stress. So let us consider a block of solid and a force F is acting on it. So when the force F acts on it then it deforms. So this is we are talking about a solid.

If you consider a liquid when a force F acts this is we are talking about a liquid when you apply a force F it keeps on deforming as long as the force exists. So in case of a liquid if you apply a force F then the solid is deformed and when the force is removed the shape is retained. The solid goes back to its original shape whereas in liquid if you apply a force then it deforms continuously as long as the force is existing.

And when the force goes to 0 in liquid the shape does not go back to its original shape. It remains in that shape and when force is again applied it continuous to deform so that is why the solids are different from liquids. Let us look at some of the properties of liquids. The different properties are kinematic properties. The kinematic properties are the properties of the flow they may also depend on the fluid properties.

So some of the examples are velocity, acceleration and strain rate.

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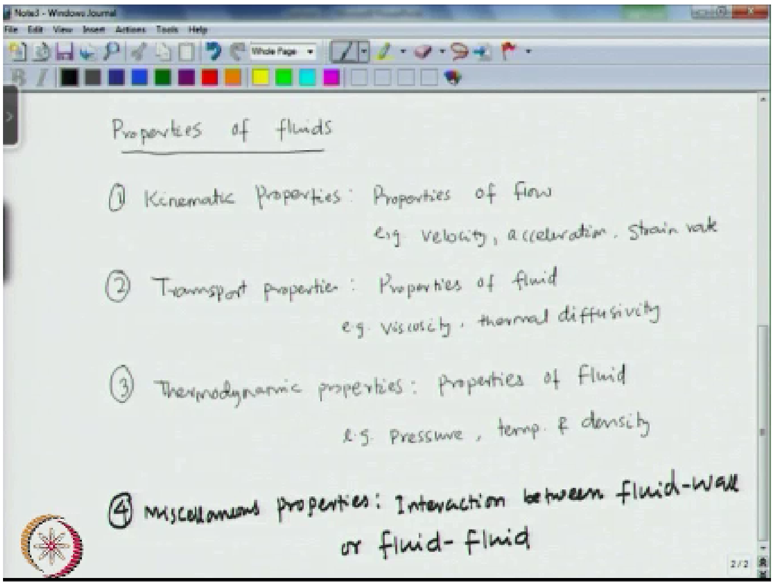

So we look at properties of fluids. So we look at first kinematic properties. Kinematic properties are basically the properties of flow and the examples are velocity and acceleration and strain rate. So these are kinematic properties. The second set of properties are the transport properties. The transport properties are properties of the fluid and these properties would affect how the fluid is transported or in case of heat transport how the heat is transported.

So we talk about transport properties. These are properties of fluid and the examples are viscosity, thermal diffusivity. Then we have thermodynamic properties. So thermodynamic properties will state the thermodynamic state of a fluid and the examples of thermodynamic properties are pressure, temperature and density. So the third set of properties are the thermodynamic properties.

So thermodynamic properties are again properties of fluid and the examples are pressure, temperature and density. Then we have miscellaneous properties. And the miscellaneous properties are the properties that of the fluid that is because of the interaction between the fluid and the wall or the interaction between fluid and fluid interaction between 2 fluids. So it is because of the interaction between fluid and wall or fluid-fluid interaction.

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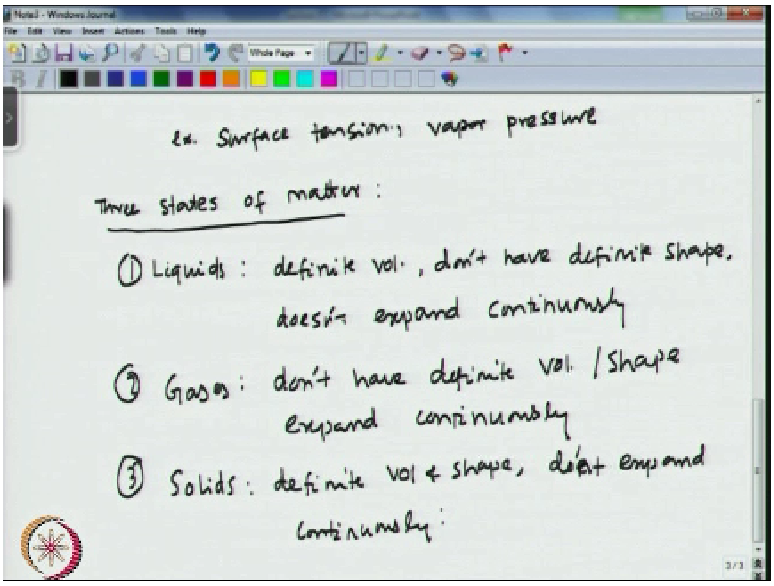

So the examples of miscellaneous properties are surface tension and vapor pressure. So now let us look at 3 different states of matter namely solid, liquid and gas. How their behaviors are different so we look at 3 states of matter. So first let us look at liquid. The liquids have definite volume. They have definite shape and they do not expand indefinitely. So the liquids have definite volume, but do not have definite shape because it takes the shape of the container and it does not expand continuously.

Next we talk about gases. The gases they do not have definite volume and they do not have definite shape and they expand infinitely. So do not have definite volume or shape and expand continuously. And third is the solids have definite volume and shape and they do not expand continuously. Now if we look at the density of the solid it is normally greater than 1000 kg per meter cube.

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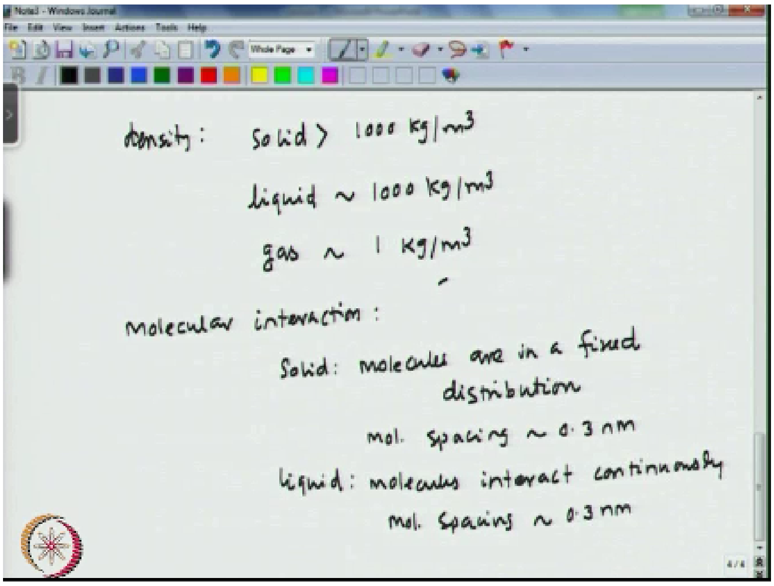

So the density if you compare the densities then the solid density is actually>1000 kg per meter cube and the liquids density is about 1000 kg per meter cube and gas density is about 1 kg per meter cube. Now if you look at the interaction the molecular interaction the molecules in the liquid they are in constant state of interaction they always interact and they move relative to each other.

The molecules in the gas they interact as and when they collide with each other briefly whereas in solids the molecules are in the relatively fixed state and they can only move relative to each other when the temperature their relative position is disturbed for example by increasing the temperature. So in solid molecules are in a fixed distribution and their molecular spacing is of the order of 0.3 nanometer.

In liquid the molecules interact continuously and their molecular spacing is also of the order of 0.3 nanometer.

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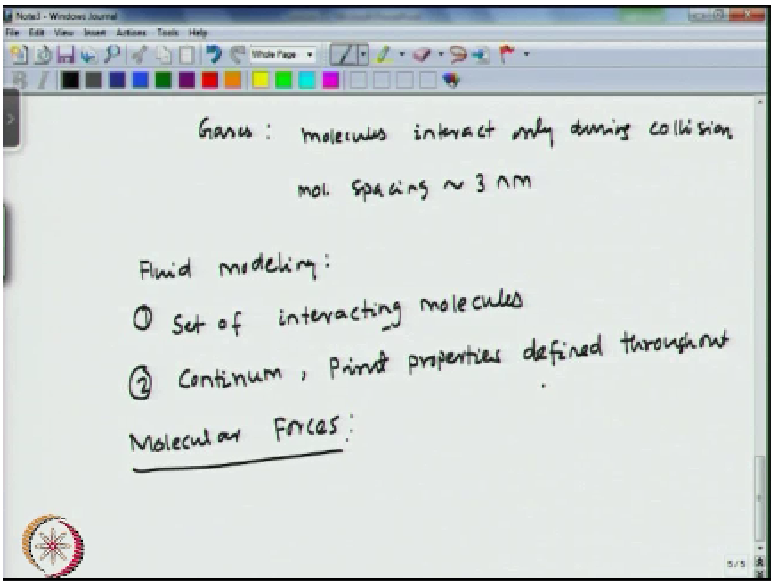

Now in gases the molecules interact only during collision and the molecular spacing is about 3 nanometer. So that is how the intermolecular distribution is in liquid, solid and gases. Now to analyze the behavior of fluids we can do it in 2 ways. In one way we can assume that they are in a state of molecules. We can consider the fluids to be distribution of molecules which are interacting with each other or we can consider the fluid to be continuous body where the point properties like pressure, density, velocity are defined throughout space.

So the fluid modeling can be done in 2 ways. One is they are set of interacting molecules or as continuum where point properties are defined throughout. So first let us consider the fluid to be as the state of molecules that continuously interact. So here we will look at the molecular theory. So we will talk about the molecular forces.

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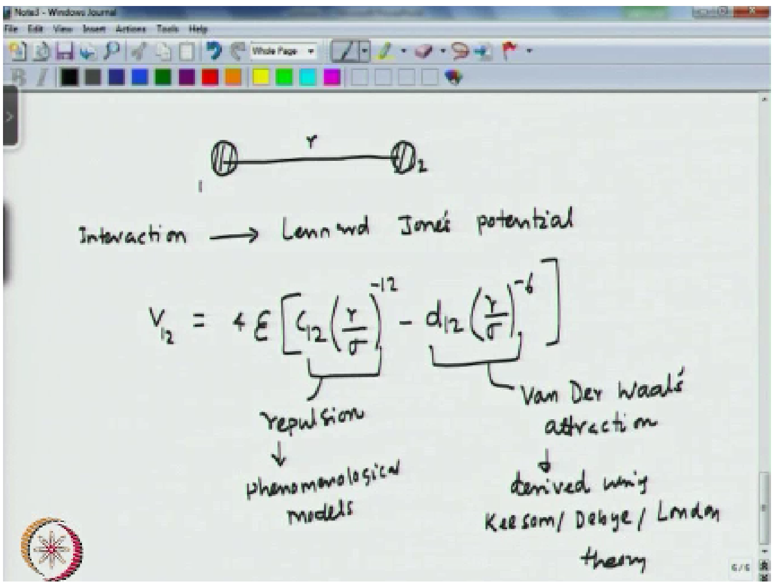

Now if we consider 2 molecules separated by distance r so this is molecule 1, this is molecule 2 there interaction is defined as Lennard Jones Potential. So the molecular interaction is defined by Lennard Jones Potential. So the Lennard Jones Potential v12 is given by 4 epsilon * c12 * r/sigma to the power -12 –d12* r/sigma to the power -6. So the first term is the repulsive term this is the repulsion between 2 molecules.

And the second term is the Van Der Waals attraction. The repulsion force can be determined using phenomenological models. It cannot be derived whereas the attraction force can be derived using different theory. There are different theories like theory Keesom theory, Debye theory or London theory. So it can be used to derive the potential between 2 interacting non reacting molecules so that is given by the Lennard-Jones Potential.

Now knowing the potential, we can determine the force that is acting between 2 molecules.

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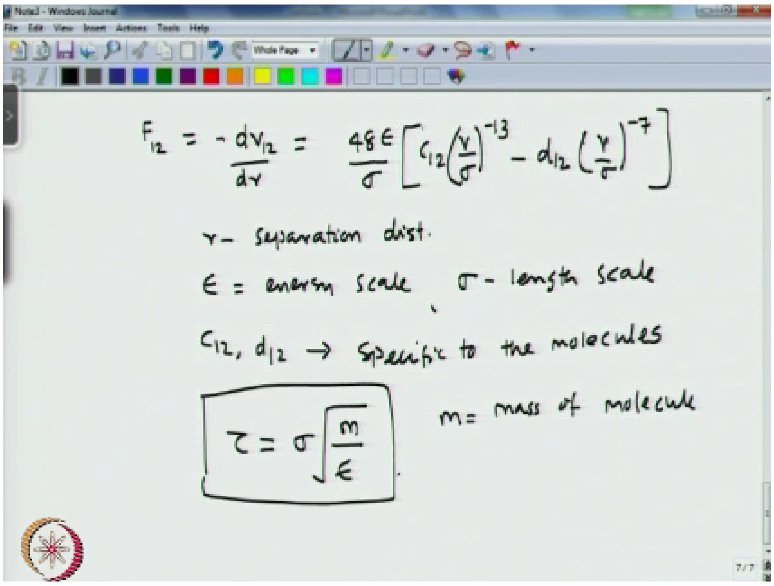

So we can determine the force F12 which is nothing, but the differentiation of the potential dv12/dr which is given by 48 epsilon/sigma *c12 r/sigma -13- d12 r/sigma -7. So here this r is the separation distance between 2 molecules. Epsilon is the energy scale. Epsilon is the energy scale and sigma is length scale and c12 and d12 they are specific to the molecules and the characteristics time scale of interaction between the 2 molecules is given by tau. So this is the characteristic time scale of interaction which is given by sigma *m/epsilon square root.

So this is the characteristic time scale of interaction where m is the mass of molecules. So when the time scale is tau then the Lennard-Jones Potential can be used to find out the force between 2 molecules.

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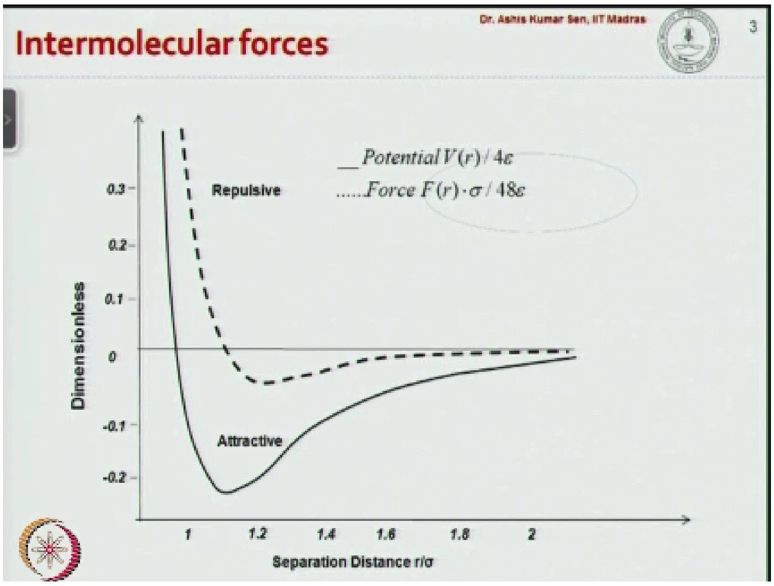

So let see how the force and the potential vary with separation distance. As you can see here as the separation distance increases the force if you look at the force when r is very less which is of the order of sigma. And sigma for fluids is about 0.3 nanometer then the force between the 2 molecules is repulsive in nature and when the separation distance increases then the repulsive force reduces and slowly the force becomes attractive.

So about r=0.9 the force starts to become attractive and for r = 1.1 of sigma it becomes maximum so the attractive force become maximum. As r is increased further then the attraction force continuous to reduce but it never reaches 0.

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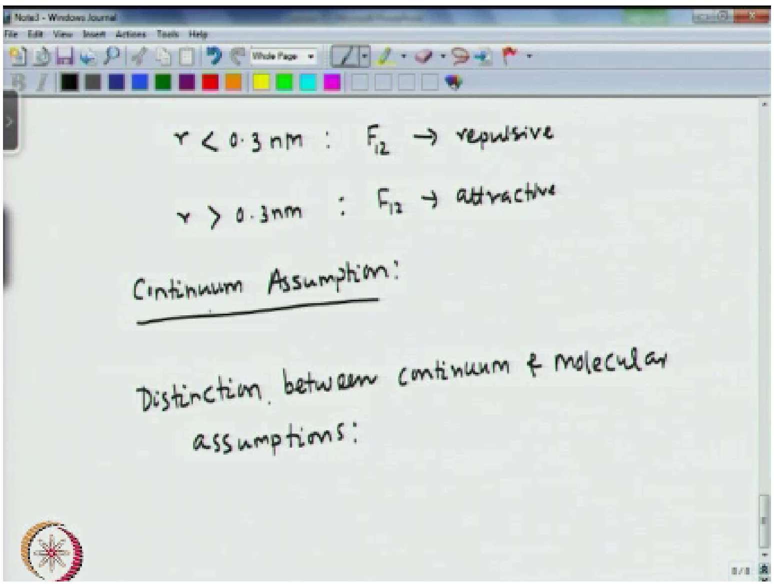

So what we see here is when r is <0.3 nanometer the interaction force is repulsive and when r is>03 nanometer then the interaction force becomes attractive. So that is what we observe from Lennard Jones Potential.

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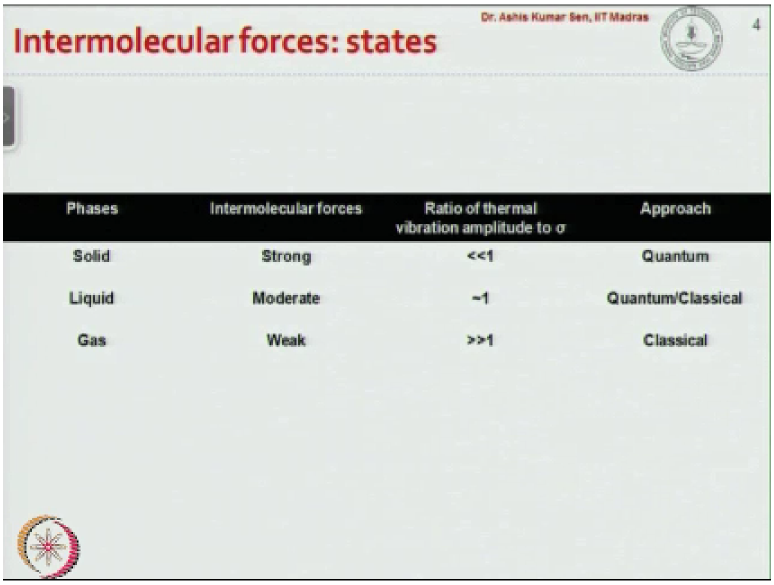

Phases	Intermolecular forces	Ratio of thermal vibration amplitude to σ	Approach
Solid	Strong	<<1	Quantum
Liquid	Moderate	~1	Quantum/Classical
Gas	Weak	>>1	Classical

Now if you look at how does the intermolecular force vary for different phases. You can see for solids the intermolecular force is very strong and the ratio of thermal amplitude vibration to sigma the characteristics length scale is going to be very small and you need quantum mechanics approach to handle that whereas in liquid the intermolecular forces are moderate and the ratio of the thermal vibration amplitude to sigma is (()) (24:10) and you would require quantum or classical mechanics to handle liquids.

In case of gas the intermolecular force is weak and the ratio of thermal vibration amplitude to sigma is>>1 and you need classical approach to handle gases. So now let us look at continuum assumptions. So we can assume that the fluid is continuum when there are lot of molecules are present in a fluidic space. For example, if you consider a channel of 10 micron size and you have water present in a channel.

There are about 30,000 water molecules present in the space. So it is almost packed with molecules in which case we can consider the presence of liquid water in a 10 micron channel as continuum. We can treat it as continuum.

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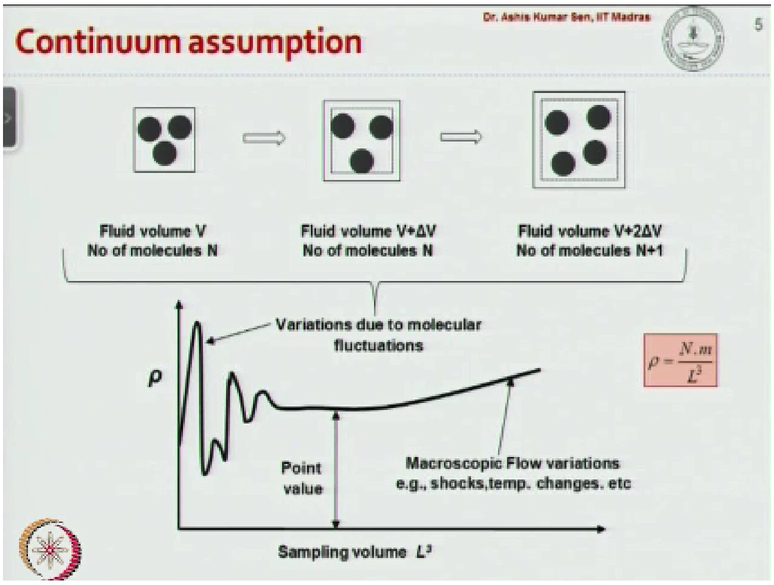

So if you look at how we can define continuum in fluidics. Here you see the variation of a point property density with the sample of volume L cube. You can see that at smaller sample volume there is lot of variation in the density in the point property. This is because when the sample volume is very small let us say in of the order of picoliter when you talk about a cube of size of the order of micron or nanometer.

When v is very small the fluid volume v is very small. Let say you have N numbers of molecules. Here we are saying that the fluid volume and the molecule volume are comparable. And if you increase the fluid volume by delta v in a small increment then the number of molecule still stays n because that increase in delta v is small compared to the volume of one additional molecule.

So you are increasing volume from v to v+ delta v whereas the number of molecules still stays n. So that would lead to sudden reduction in density because you are increasing volume without increasing the mass of the molecules. If we increase the volume further from V+ delta V to V+2 delta V then suddenly may be one molecule can be added into the volume. So suddenly you have n+1 number of molecules with equal increment in the volume.

So there will be a sudden increase in the density so that would lead to increase in the density. So for that reason when the volume under consideration or the control volume is comparable to the size of the molecule the volume of the molecule then there are lot of molecular fluctuations so that leads to fluctuation in the point properties that we see in the left side of the plot.

And when the sample volume is considerable these variations are averaged out and you get almost constant value of density which is called point value and when you talk about very large sample volumes what happens is if the volume is very large then local fluctuations tends to occur. For example, you have local heating of the flow that would lead to change in the density at a particular location.

So in that case also we cannot consider the flow to be continuous. The assumption that flow is continuous breaks down. So next we look at the distinction between continuum and molecular assumptions. So we look at nitrogen gas and liquid water.

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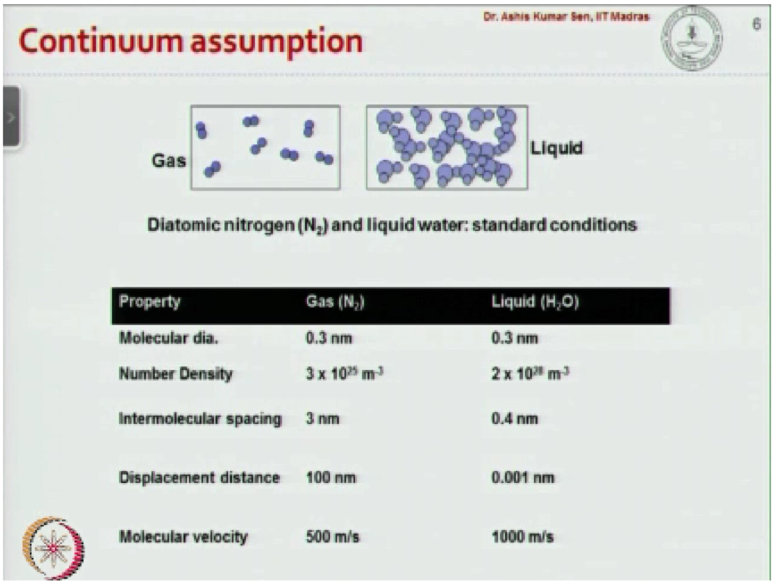

So as you see here to describe the continuum assumption we consider diatomic nitrogen and liquid water at standard conditions. So the different properties that is shown here one is the molecular diameter the molecular diameter of nitrogen is about 0.3 nanometer which is the same as the molecular diameter of water. The number density of nitrogen is 3*10 to the power 25 per meter cube and the number density of the liquid water is 2*10 to the power 28.

The intermolecular spacing the spacing between the molecules in case of nitrogen is 3 nanometer whereas in case of liquid it is 0.4 nanometer about 10 times less. The displacement distances the molecules between collisions is about 100 nanometer for gas and it is about 0.001 nanometer per liquid. So the liquids are in constant state of interaction. If you look at molecular velocity for the gas it is 500 meter per second and for liquid, it is about 1000 meter per second.

Now let us differentiate between the molecular and continuous behavior by considering 2 fluids one is liquid water and the second one is diatomic nitrogen. For statistical confidence we will consider about 10 to the power 4 number of molecule. So that we have enough molecules to know their behavior.

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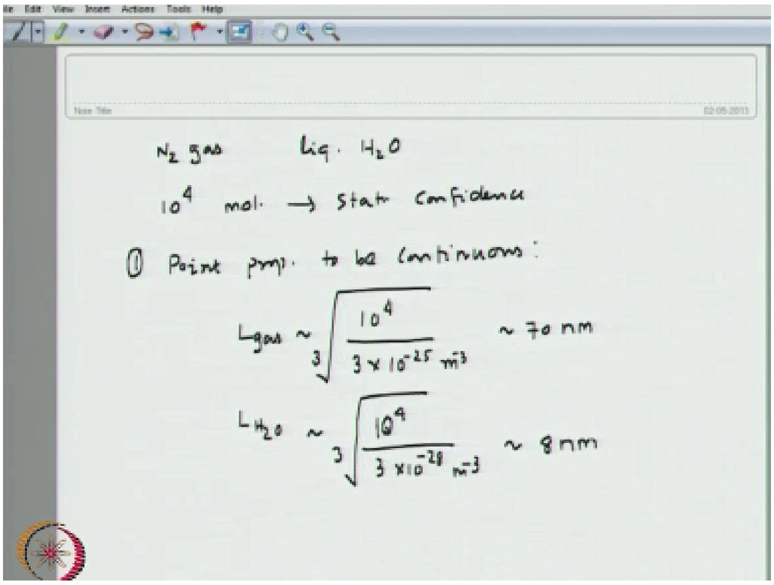

So we will consider nitrogen gas and liquid water and we would consider 10 to the power 4 molecules for statistical confidence. Now first to have the point properties to be continuous we would determine what should be the point volume, what should be volume of the space so that we can consider either the liquid to be continuous and the gas to be continuous. To consider the gas to be continuous the length scale of the gas has to be 10 to the power 4 molecules.

We are considering and the molecular density of the gas is 3*10 to the power -25 per meter cube. So take the cube root we get 70 nanometer. So if we consider gas cube that has dimension 70 nanometer each side then we can expect that the point properties will be continuous. For liquid, for water it will be 10 to the power 4/ number density is 3*10 to the power -28 per meter cube and if we determine that it will be about 8 nanometer.

So if we have liquid water in a point volume that has the cubic size of each side 8 nanometer then we can expect that the liquid water is still continuous.

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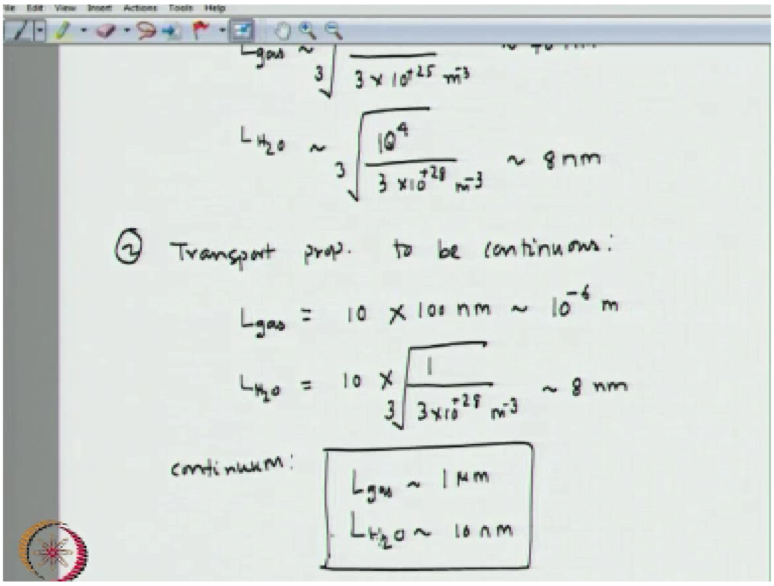

Next we will determine if we talk about the transport properties. Transport properties to be continuous we expect that for example viscosity is continuous then we say that the volume of the cube would be about 10 times the distance of travel of the molecule. So in that case the L gas would be 10 times the distance the gas molecule would travel which is about 100 nanometer is the separation distance.

So 10*100 nanometer which is about 10 to the power -6 meters. For liquid water for water the molecules are in constant state of interaction. So in that case the separation distance will not be a good parameter to establish its length scale at which it will be continuum whereas the size of the molecule would be a good parameter to establish whether the liquid water is going to be continuous.

So same way we consider that it is 10 times the size of the molecules which is 1/3*10 to the power +28. So these are number of (()) (35:56) so which will be about 8 nanometer. So what do we see here. We see here that for gas to be continuous the length scale of the flow has to be at least one micron and the length scale of the liquid has to be at least about 8 nanometer or 10 nanometer.

So for continuum behavior gas has to be 1 micron and water is about 10 nanometer. So this is very important to understand in which case we are going to expect continuum behavior if we are talking about liquid flow, flow of water through 2 parallel plates and the separation distance is less than 10 nanometer then we can consider the flow to be in molecular regime. We cannot apply the continuum governing equations to solve for the flow.

Whereas in case of gas flow if the separation distance is above 1 micron R then only we would expect that the continuum behavior is expected. So that is very important to understand. So having said that let us look at the continuum fluid mechanics. As we know that in most micro-scale flow situations the separation distance or the length scale of the flow is going to be well above 10 nanometer.

We can say that for most of the liquids flows the flow can be treated as continuum.

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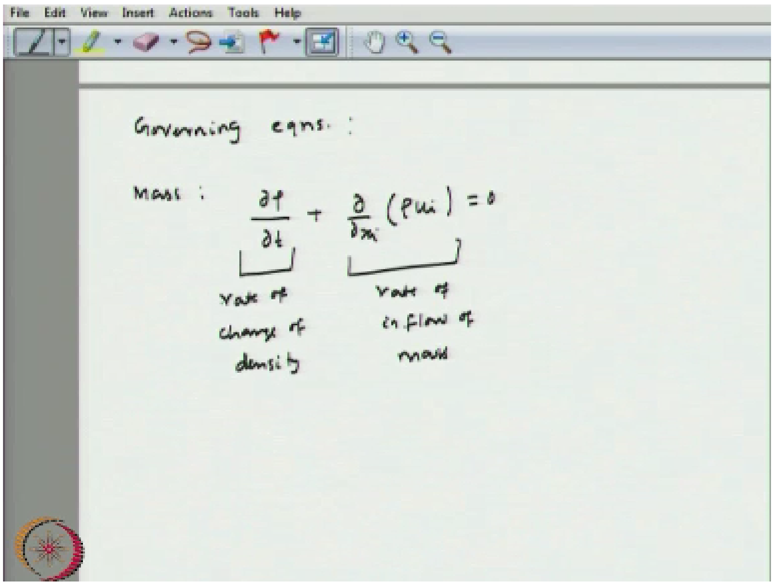

So with that let us talk about the governing equations for the fluid flow at micro-scale governing equation namely the mass conservation equation can be written as follows del rho/del t+ del/del xi* rho ui is 0 and the first term is the rate of change of density. The second term is the rate of inflow of mass.

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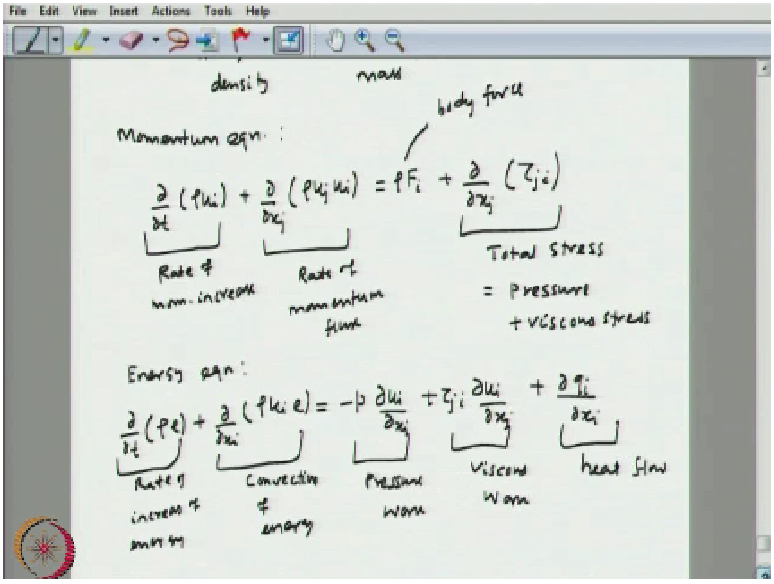

Next we can write the momentum equation. Momentum equation which is del/del t *rho ui+ del/del xj* rho uj ui= rho Fi+ del/del xj* tau ji. So this is the rate of momentum increase, this is the rate of momentum flux, this is the body force and this is the total stress and this total stress will have the pressure component + viscous stress. We can write the energy equation del/del t*rho e+ del/del xi * rho ui e=-p* del ui/del xi+ tau ji* del ui/del xj+ del qi/del xi.

So this is the rate of increase of energy. This is convection of energy. This is the pressure work, this is the viscous work and this is the heat flow.

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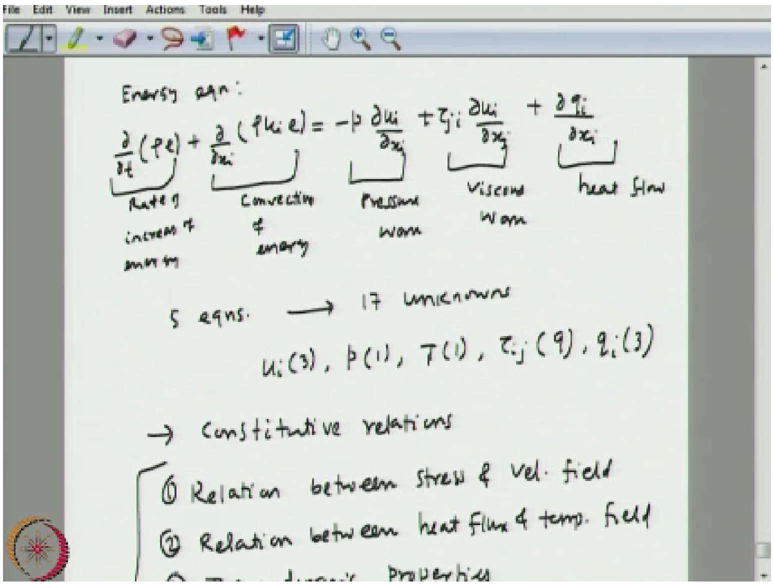

So if you look at here. We have 5 equations and we have 17 unknowns. So those unknown are we have ui 3, we have pressure, we have temperature and we have the stress tensor, we have 9 components and then we have qi 3 components. So we have totally 17 unknowns and

5 equations. So to solve we require the constitutive relations that means we need the relation between the stress and velocity field.

We need relation between heat flux and temperature field and we need to express thermodynamic properties. So that is what we need to solve the 5 equations the mass, momentum and energy. There are CFD codes available which can solve these equations and in some special cases where the physics of the problem can be simplified and these equations can be simplified to a form which can be solved analytically we can obtain the solutions also.

So with that first let us try to look at gas flows then we will move on to liquid flows.

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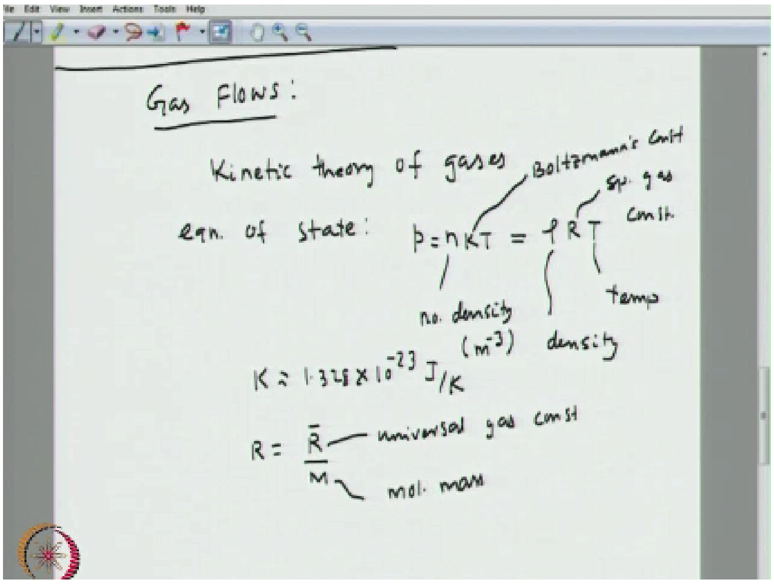

So first we try to look at gas flows. So the gas flows can be described by the kinetic theory of gases and in order to apply the kinetic theory of gases one requirements is that the molecules of the gases should move in a straight line between the collision so that is the assumption that we are making. So under that assumption we are able to apply the kinetic theory of gases where we first look at the equation of state which is p=nkT or also written as rho RT where n is the number density how many molecules we have for you need volume.

Number density is per meter cube. K is the Boltzmann constant and T is the temperature, R is the specific gas constant and rho is the density. And this Boltzmann constant k has a value which is 1.328*10 to the power -23 joule per Kelvin. The specific gas constant R can be written as universal gas constant/molecular mass. So this is universal gas constant and this is the molecular mass.

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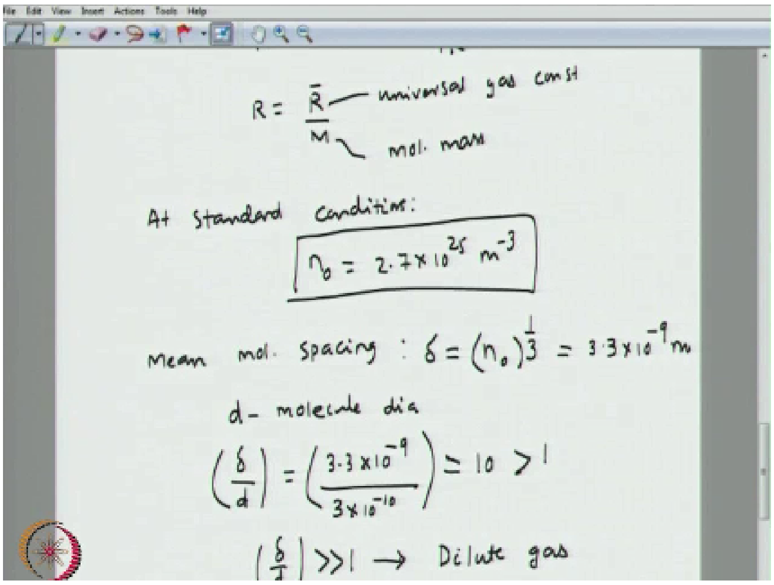

Now at standard conditions meaning the temperature is 273.15 and the pressure is 101.325 kilopascal. We would have the number density n0 to be 2.7* 10 to the power 25 per meter cube. So that standard conditions we have these many number of molecules per meter cube. So we can find the mean molecular spacing. So the mean molecular spacing will the cube root of that.

So delta will be n0 to the power 1/3 which will be=3.3*10 to the power-9 meter. So the mean molecular spacing on a standard condition is about 3 nanometer and if we can compare the spacing between the molecules with the diameter of the molecules and if the diameter of the molecules to the spacing ratio is going to be very small then the gas is called dilute gas. So if d is the molecule dia and the ratio of delta to d.

For example, in case of nitrogen this is going to be 3.3*10 to the power -9. So diameter will be about 3*10 to the power -10. So this will be about 10 which is> 1. So if delta/d is>>1 then it is called a dilute gas. So in dilute gases you would have only 2 molecules colliding with each other at one time. Many molecules or more than 2 molecules colliding with each other is not possible.

So next we look at 3 different important parameters in the gas flows. One is the lambda which is called the mean free path.

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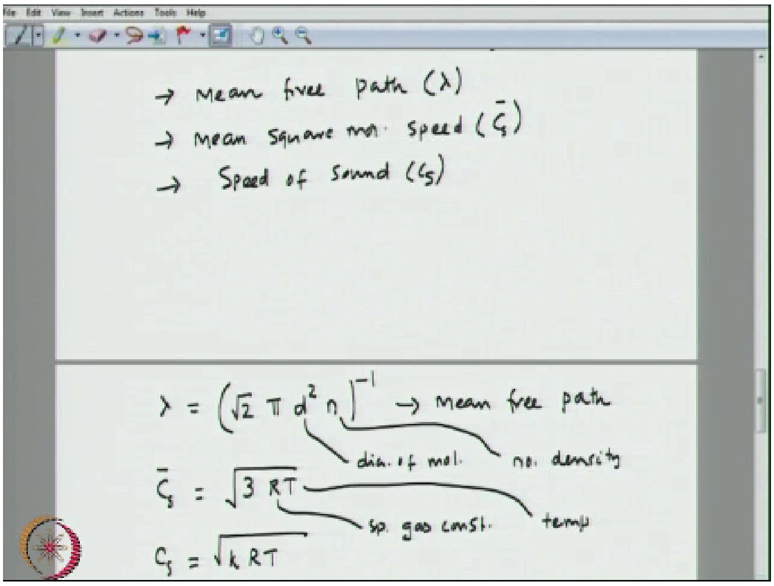

So mean free path we look at 3 different parameters here one is mean free path which is lambda. We will also look at mean square molecular speed which is denoted Cs* and we would also look at speed of sound which is Cs. So the mean free path lambda can be so the mean free path is the distance that a molecule travel between 2 successive collisions. So lambda can be expressed as follows.

Lambda is given by square root of 2*pi* d square n to the power -1. So this is the expression for the mean free path. So the molecular speed Cs mean square molecular speed can be written as 3 R*T and the speed of sound can be written as square root of k R*T. So here the d is the dia of molecule and n is the number density how many molecules per meter cube. R is the specific gas constant and T is the temperature.

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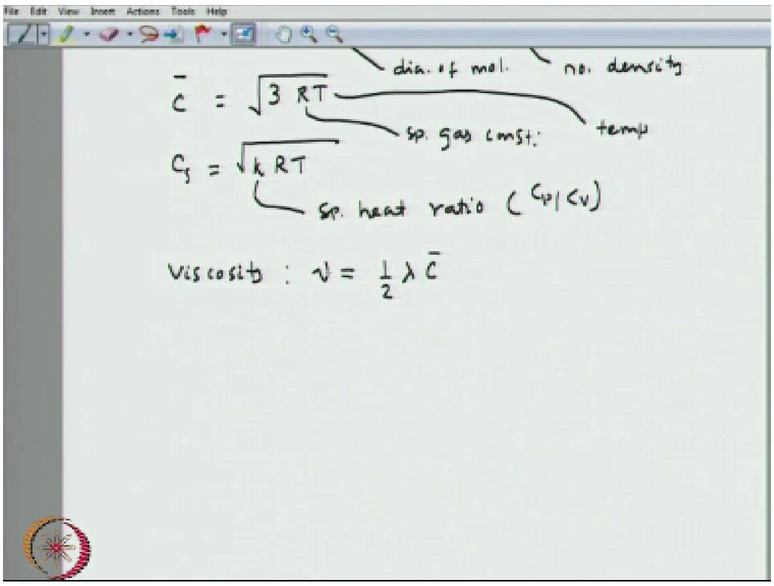

This is specific gas constant and K is the specific heat ratio that is Cp/Cv and viscosity can be written as nu will be nu will be 1/2*lambda* c bar which is the speed of the mean molecular speed. So this is actually c bar not Cs which is denoted by c bar there is a correction here also. So here we write c bar. So using this expression the viscosity can be related to temperature and pressure as the mean free path lambda is a function of pressure.

And c bar the mean square molecular velocity is a function of temperature. Next let us look at some of the dimensionless parameters in gas flows. We will look at Knudsen number, we will look at mach number, we will look at Reynolds number and we would have see how they are related.

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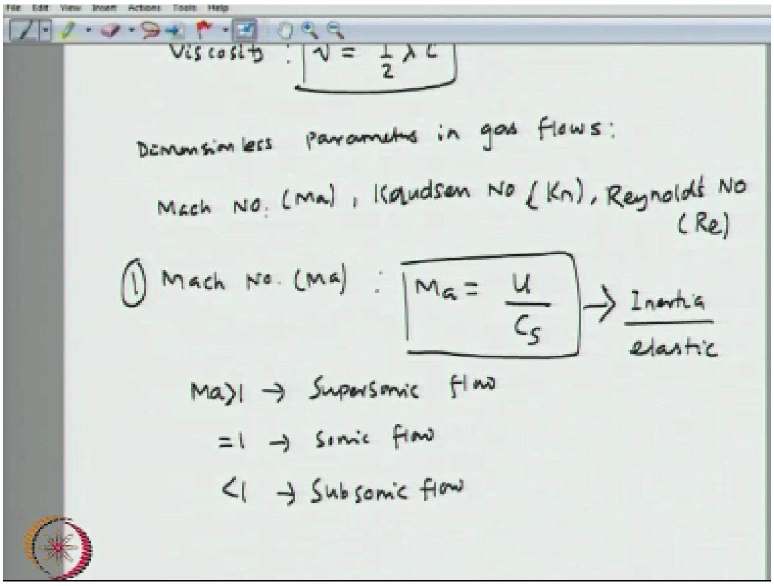

So let us look at dimensionless parameters in gas flows. First is the mach number denoted by Ma then you have Knudsen number is denoted by Kn and then you have the Reynolds number Re. So first let us talk about mach number Ma. Mach number is the ratio of the velocity of a fluid to the velocity of sound in a median. So Ma is u/Cs and it is also referred to as the ratio between the inertia force to the elastic force.

So ratio between inertia to elastic. And depending on the mach number we can categorize the flow where the flows where the mach number > 1 which is known as supersonic flow when they are of the order of 1 they are sonic flows and when mach number<1 they are subsonic flows. So mach number>1 supersonic flow. When mach number=1 sonic flow and<1 subsonic flow.

So we can say let say for example gas is flowing through a channel and we know that gas is compressible, but within the channel if there is no variation in the density we can consider the flow to be incompressible that is a very important to concept in fluid mechanics or in gas dynamics. The fluid could be compressive, but if there is no change in the density inside the device the density is not varying.

We can consider the flow to be incompressible.

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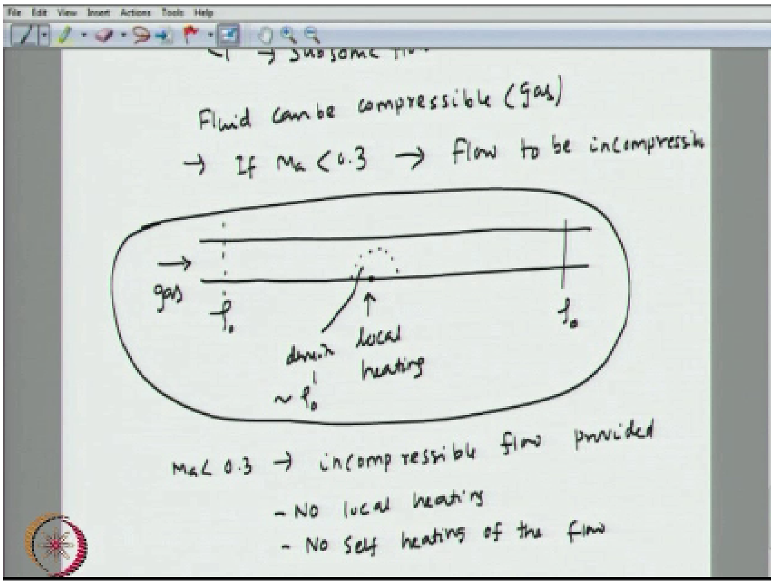

So fluid can be compressible. Let us say gas, but if the mach number is<0.3 then we can consider flow to be incompressible. So let us consider a flow through 2 parallel plates and let say gas is flowing and density here is rho 0 and is continuously staying rho 0 till this point and so in that case even if gas is compressible the flow could be considered as incompressible.

And most likely the mach number if the mach number is<0.3 we can still go ahead and use the governing equations that is applicable to incompressible flow to this situation. Provided few other conditions are satisfied for example in this case if we have let say somewhere there is local heating of the flow if you have local heating then around here around this region the density may rho 0 dash which is different than rho 0.

So in that situation if you are analyzing this domain we cannot say that the flow is incompressible. So in addition to satisfying the condition that mach number is<0.3 there should not be any local heating of the flow. There are other cases for example if there is a gas flowing through very thin parallel plate and the viscosity is considerable then there will be viscous heat generation and there will be heat loss.

There will be self heating of the gas. So in that case also we cannot consider flow to be incompressible. So normally if mach number<0.3 we consider incompressible flow provided there is no local heating, no self heating of the flow. So that is the condition even if the mach number<0.3 there should not be any local heating, there should not be any viscous heat generation.

So with that we move on to talk about what is the Knudsen number.

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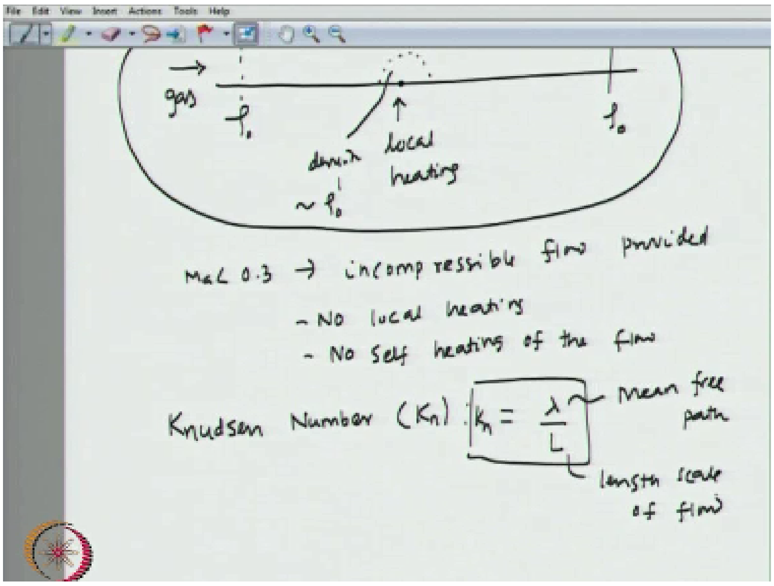

So we will talk about Knudsen number which is denoted by Kn. So Knudsen number is defined as the ratio between the molecular length scale the mean free path lambda and the length scale of the flow. So Knudsen number is lambda/L. So that is lambda is the mean free path and L is the length scale of flow. Now depending on the value of the Knudsen number we can categorize how rarified the flow is.

So there are different ranges of Knudsen number we can come up with. If Knudsen number is<0.001 then we can treat the flow to be continuous. We can apply the Navier Stokes Equation and the boundary condition no slip boundary conditions. If the value of Knudsen number is between 0.1 to 0.001 then we can still apply Navier Stokes Equation, but with slip boundary conditions.

And if Knudsen number is between 0.1 to 10 then we are in the transitional regime where we need to modify the Navier Stokes Equation in order to use it and if the Knudsen number is>10 we get into molecular regime.

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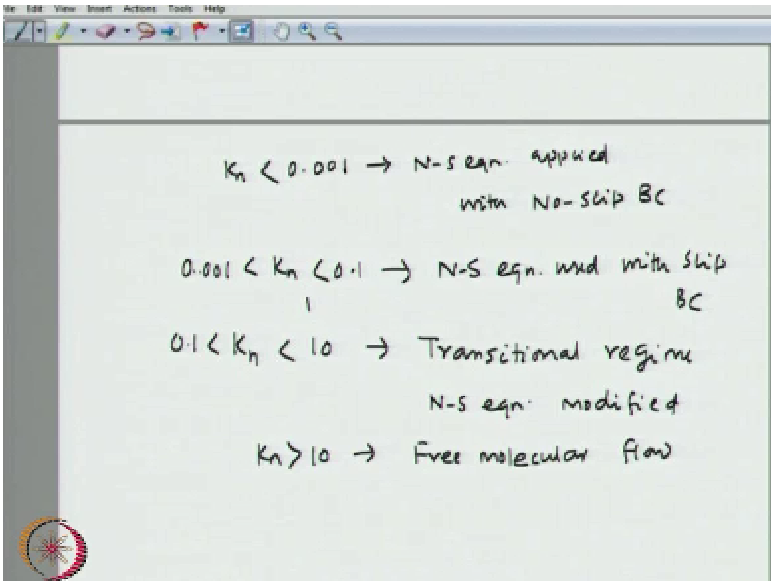

Knudsen number is<0.001 can say that Navier Stokes Equation applied with no slip and 0.001 if Knudsen number is between 0.001 to 0.1 then Navier Stokes Equation used with slip boundary conditions and if Knudsen number is between 0.1 to 10 then we are in the transitional regime where Navier Stokes Equation modified and if Knudsen number is>10 then 3 molecular flow.

So next we talk about Reynolds number is the ratio of the inertia to viscous force.

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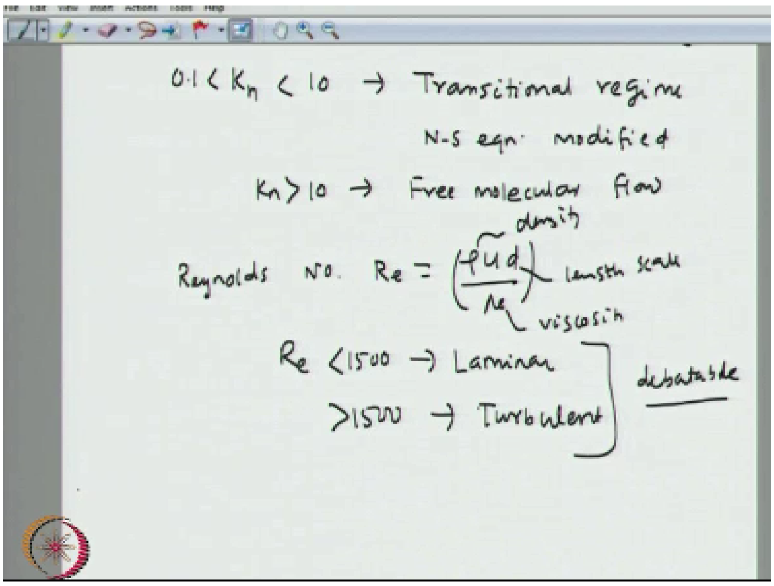

Reynolds number is denoted by Re which rho u d/nu and depending on the value of the Reynolds number we can categorize the flow. If Reynolds number<1500 we can say lamina Reynolds number>1500 and say this is going to be turbulent. Although at micro-scale this is debatable so which we will be discussing later on. So here this is density, this is length scale and this is viscosity and U is the velocity. So now we can relate the mach number.

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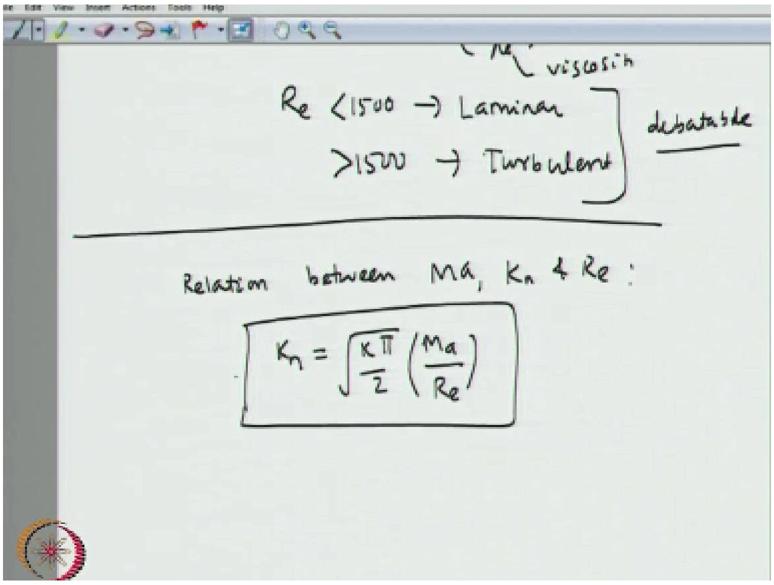

Relation between mach number, Knudsen number and Reynolds number. So the relation is going to be this. The Knudsen number will be=k*pi/2 square root* mach number divided by Reynolds number and we stop here.