Micro and Nanoscale Energy Transport
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Lecture – 21
Kinetic Theory of Energy Carriers Part 2

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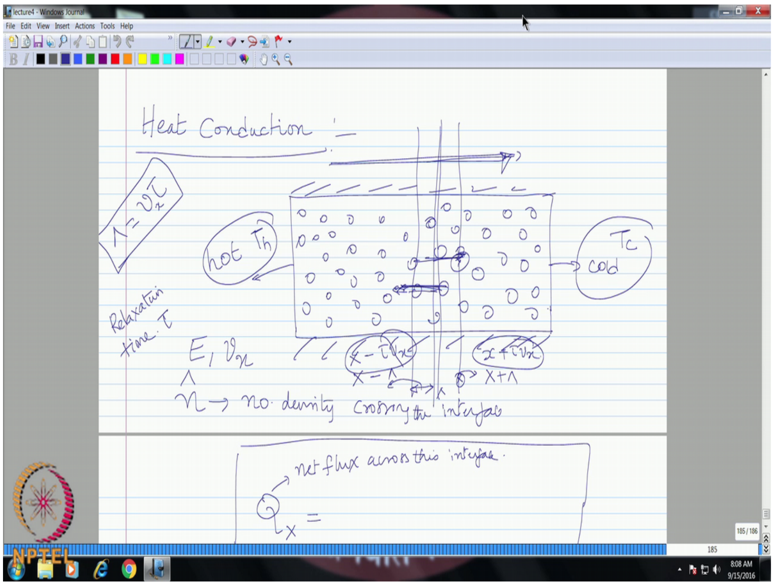

Good morning, we will continue our discussion related to the transport of phenomena, the first thing that we started yesterday was the transport of heat, that is the heat conduction through for example, gas molecules, this can also be extended to other energy carriers like phonons or electrons considering them as phonon gas and electron gas respectively.

So we have also I mean said that you know this way of (Refer Time: 01:03) the gas molecules using the kinetic theory is a little bit approximate way, but never the less gives us some useful expressions for deriving the relationship between thermal conductivity and other molecular characteristics. So therefore, the first example that we have taken is in the case of heat conduction.

So we considered a system or a box, one end of the box is at higher temperature t h and the other end is at colder the temperature and we consider the system of gas molecules an ideal gas and to apply the kinetic theory, we consider an interface somewhere inside the system at a location of what we call x and in order to look at heat conduction, what we ideally need to know is how far a gas molecule can travel across this interface before it collides with the neighboring molecule and transfers its energy, so this is how the conduction really happens at the molecular level.

So therefore, we identified interfere x, and therefore the distance travelled by a molecule across this interface before it collates with another molecule will be x plus, delta x or x minus delta x where delta x will be the mean free path of the molecule. So therefore, we also wrote down before this, that is how we are going step by step. So, the actual kinetic theory starts here, but to understand how to now calculate the mean free path.

So, earlier we will do this derivation and we estimated the mean free path for the ideal gases through this particular relationship here. So ones you know the mean free path, here the mean path requires knowledge of temperature and pressure. So therefore, before that we had identified the relationships for calculating the temperature and pressure. So fundamentally if you are looking a temperature and pressure of these gases. So they are functions of the kinetic energy of the gas molecules.

So ones you know them you calculate the mean free path and therefore ones you know the mean free path, now we apply the kinetic theory for the transport process. So ones mean free path is define you can relate the mean free path to the relaxation time, that is the basically we are converting a lengths scale into time scale. And therefore we can write these left and the right ends where the molecules can cross this interface and travel till it collates with the neighboring molecule as x plus tau in to v x and x minus tau in to v x.

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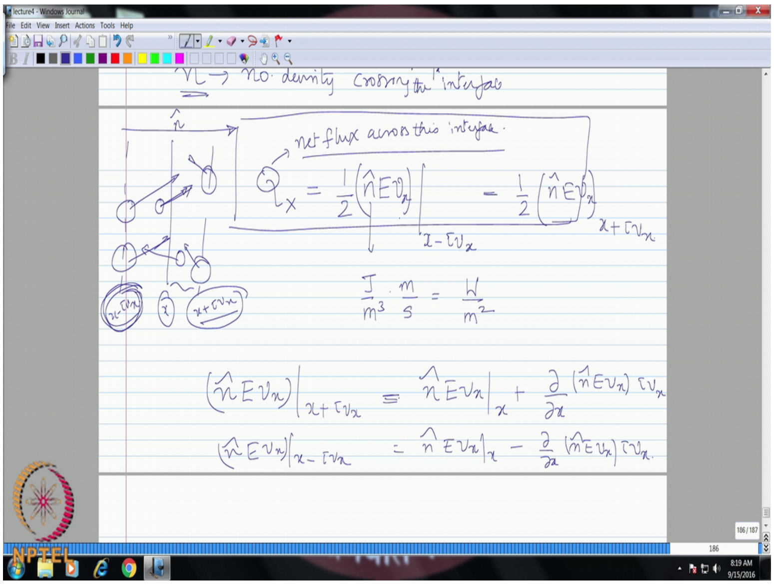

Now, you know if you are looking at the propagation of gas molecules here. So let us redraw this focus this towards this interface x again. So, you are talking about an interface x, x plus tau t x, x minus tau v x. So there are molecules which are crossing the interface and travelling towards the right and there are also molecules crossing the interface travelling towards the left. Therefore look at a number density that is n cap, say number of molecules per unit volume and if you say that these are present right now at somewhere around this interface.

So, there is an equal probability that half of these molecules can travel towards the right and they can reach x plus tau v x before colliding with the other molecule and half of these can travel towards the left, before colliding with the other molecule at x minus tau v x. therefore if you fix this and look at from the perspective of x minus tau v x, x plus tau v x, we can say that the molecule which is travelling crossing this interface and travelling towards the right is actually 50 percent of it is or half of it is coming from this side, and half of it is coming from this side. So just to calculate the net flux of molecules which are basically going from left to right. So this is the direction of the heat conduction.

So, we can consider that since the molecules across this interface, half of them can come from the right, half of them can cross and go towards the left. So there is an equal chance that 50 percent of the molecules here are going towards the right and crossing this interface and 50 percent of the molecules at this point go towards left and cross this particular interface.

So, therefore, you have contribution of molecules from the hot side, which are moving towards the interface and also from the cold side which are moving towards the interface, but what we need is that the net flux of heat should be transfer from the left to the right the end. So based on this we can say that, the net flux across this a particular interface at x will be half of the number density of molecules which are actually located at x minus tau v x, these are the ones which are moving towards the right, minus half of what we have at x plus, tau v x, which are moving towards the left.

So, the net difference between this molecules towards the right and left the net difference in the energy, now this is just the number of molecules, but what we need to now calculate is the energy flux that is transported by these molecules moving towards the right, energy flux towards the left and then we have to show that the net energy flux is moving from the left to the right.

So, therefore, how do you calculate the energy flux; this is the number density here, from this how do we estimate suppose your E is the energy of the molecule, now could be the translational kinetic energy if you just consider monatomic gas. And v x is the velocity which this molecules are moving in the translational direction. So, if you multiply this E times v x, now you will get the units of energy flux what is the unit of energy flux?

Student: Joule per meter square.

Joule per meter square, so this is something per number per meter cube. So, number of molecules times the energy per molecules. So, this is joule per meter cube in to meters per square second, this is watt per.

Student: Meter square.

Meter square. So, if you look at your Fourier heat conduction law q is equal to minus k d t by d x q is a watt per meter square. Therefore, similarly at x plus tau v x we have, the energy flux which is bringing the molecules from the right towards the left to cross this interface. So this is the basic idea behind applying the kinetic theory. Now from this what we can do is that, we can use the tailor series approximation therefore, so we can write down the flux of energy at the point x plus tau v x in terms of the flux at x. Similarly we can estimate the flux of the molecules at x minus tau x from the flux at x. So, this can be written as n cap E V x at x plus d by d x of n cap E V x in to this distance which is nothing but, tau V x that is your main free path, high higher order terms can be neglected. Similarly n cap E V x, x minus, so can you please calculate this net flux form this Taylor series.

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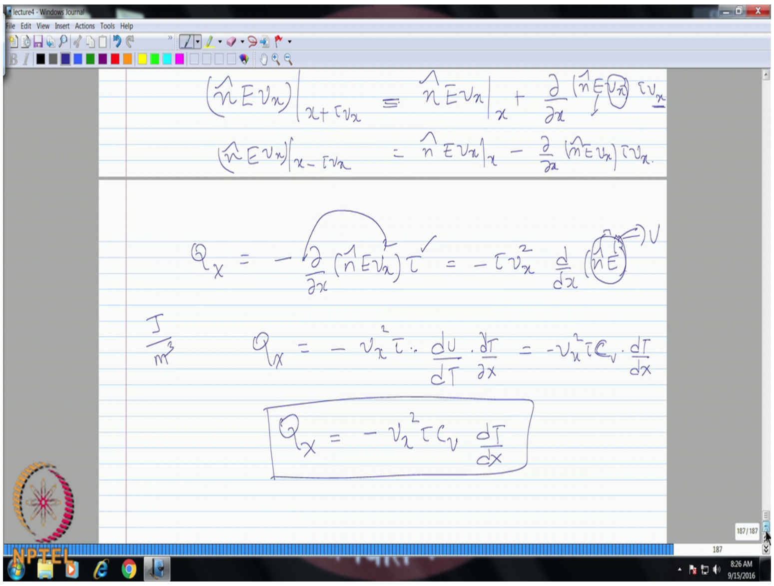

Student: (Refer Time: 11:24).

No this is the energy of a molecule that is your half m b square, but what we are looking at the total energy of these molecules at this location, so that will be different. So the velocity is function of what temperature. So, we have shown this from, if you just look at yesterday's derivation. 3 by 2 K B T is equal to half m v square.

So, that is the total kinetic energy is equal to 3 by 2 K B T. So therefore, depending on the temperature the local velocities and therefore the kinetic energy will be different, that is that is how the energy transport is happening. So therefore, if you are looking at the molecules which are coming from the x minus tau v x and crossing this interface, so in total they will have a higher kinetic energy compare to this and that is how the net flux can go from the left to the right. So, although they are just half m b square all the molecules, but the value of v x will be different depending on the temperature. So we have minus del by del x, n cap E v x in to yeah v x square tau.

So therefore, we can just relaxation time is a constant and what we can also pull out. So, we have just a moment. So, we have tau v x here, v x here and now we have to make a small approximation for the sake of simplification here, that when we are doing this we have to assume that, although this energy is your internal energy that is your translational energy which is again related to velocity and that is function of space. We are assuming that the flux of this is actually transported by this velocity, in this velocity is kind of fairly reasonably uniform.

So therefore, to make this analysis a little bit simpler, this v square will be pulled out of the derivative, but this energy cannot be of course, this energy is nothing, but the internal energy or your kinetic energy flux. Although that is a function of, molecular level it is a function of half m v square and that velocity is a function of temperature. So, for the sake of simplification right now will pull this e square out of the derivative here, so we will have tau v x square and we have d by d x, but this energy what we have written will be a function of, of course x otherwise that is not transport.

So, this is what we are going to do now and then we will split this as minus v x square tau into. So basically this is your number density times E. So the unit of this will be joule per meter cube. So, this is joule per meter cube is what? Volumetric energy so, this is therefore, replaced by U. So therefore, this can be written as d u by d x which can be rewritten as d u by d t times d t by d x because U is a function of t this K B T is equal to half m v square. Therefore, we are rewriting like this and d u by d t the volumetric internal energy derivative of this with respect to temperature this is your volumetric heat capacity.

Therefore we can write this as V x square, tau times C v into d t by d x. I mean strictly speaking you might ask this v should not have been pulled out, because fundamentally you know half m v square is equal to K B T, the velocity is might be different. Therefore, there is the gradient of velocity, but this is a little bit simplistic assumption, we pull out the velocity outside the derivative assuming I mean the energy is one, which is actually having a gradient. Otherwise then this becomes quite difficult, to bring it to the form of the Fourier heat conduction equation. Now compare this to the Fourier heat conduction equation.

So, now right now from kinetic theory says that, your heat transfer rate is your equal to V x square, tau, C v, d t by d x this is your heat flux and compare this to your Fourier heat conduction equation you have Q x is equal to minus k, d t by d x.

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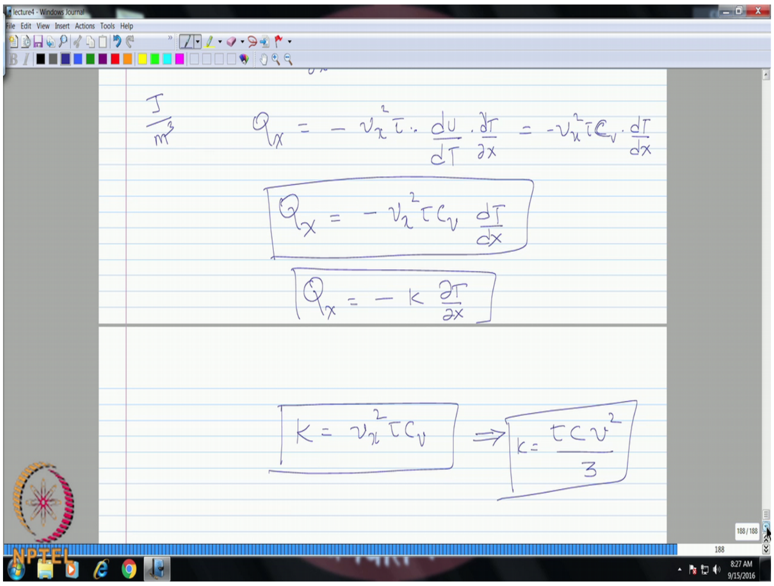

So, now we have brought it to this form. So therefore from this what can we say about K, this is equal to v x square, C v, tau. So therefore, if you want to rewrite this in terms of the velocity in net total velocity v, we can replace v x with v by 3, V square by 3. So, therefore, this can be written as tau c into v square by 3.

So, this is how now molecular level you have the velocity of the gas molecules, the relaxation time, so these are now intern governing your transport property called "Thermal conductor". So, the same thing can be extend to other energy carries phonon gas, you have to use a corresponding relaxation time of the phonon gas corresponding velocities electron gas.

So, you can use a parallel treatment, therefore you can determine the corresponding thermal conductivities of electron gas. So therefore, you are talking about now metals. So, you want to estimate the thermal conductivity of this metal. So, you are now looking at the electrons and therefore you put the corresponding value of volumetric heat capacity of this particular substance of this material and how is volumetric heat capacity where is it coming from.

Student: (Refer Time: 20:15)

From the earlier statistical thermo dynamics, we have derived the expression for volumetric heat capacity for electrons, phonons molecules. So, if the electron is the majority charge carriers you have to use them. So, again if you go back and see for electrons, what was the relationship for C e we had a relationship like this.

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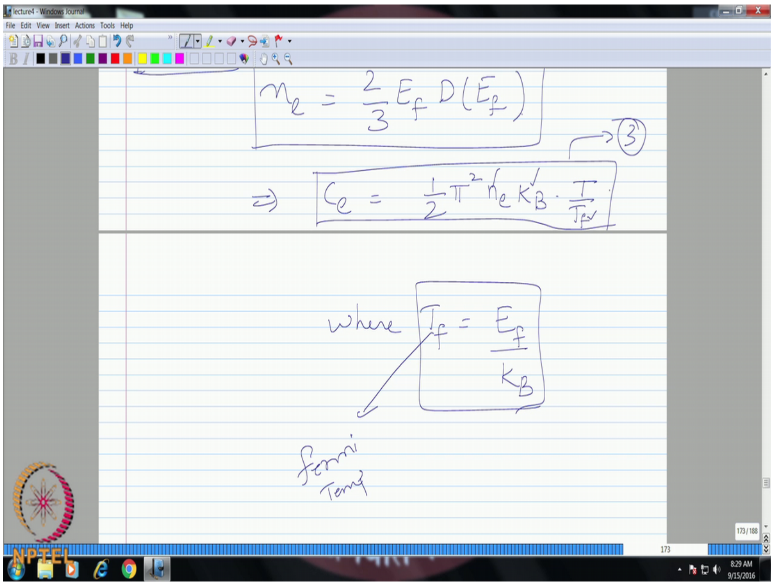

So, function of linear function of temperature. Therefore, now what is going to govern particular material, Fermi temperature and number density of the free electron, correct? That is going to differentiate different materials and depending on that your heat capacity is going to change. Once you estimate your heat capacity from the statistical thermodynamic put that into this expression, now you also know the relaxation time and the velocity and therefore, this will give you your thermal conductivity.

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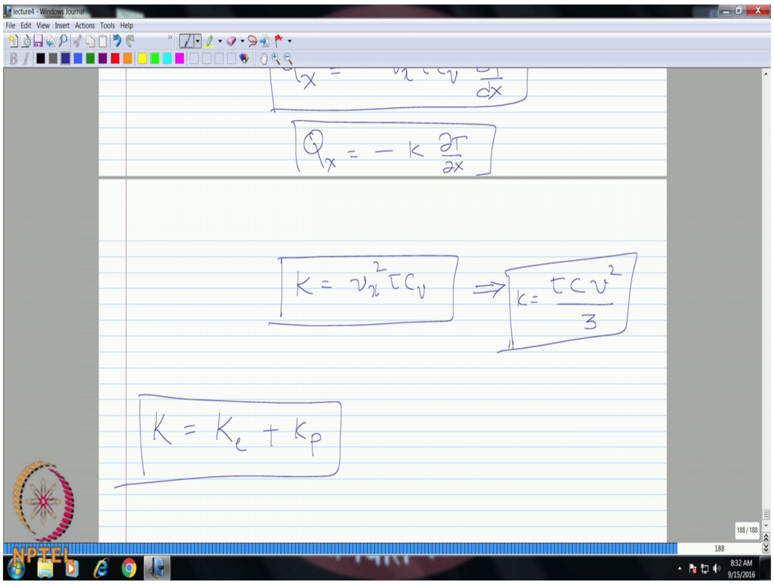

Student: sir (Refer Time: 21:29)

So, if you are the looking at some semi conducted device now. So, you have contribution from phonons primarily also electrons correct. So, in that case how do you do this? Therefore, you have to have 2 contributions to k the thermal conductivity will come from one contribution from electrons the other from phonons and you have to sum these 2 contribution this will give you a total thermal conductivity. So, you are in semi conductors your electron contribution may be small, compare to the phonons, but still if you want to get the total conductivity you have to sum these 2 components.

So, therefore, individually you have to estimate for the electrons, phonons and then sum these 2 components together right. So, may be to also give an example; you can therefore, study in the case of say air take the case of air calculate the thermal conductivity of air at normal standard atmospheric temperature and pressure, and then you can also do this for the case of metals with electrons, you can apply this to calculate the thermal conductivity of certain material metal for example,. So, you can directly see, so, in which case the conductivity will be higher. So, if you are thinking about the relaxation time. So, this is directly propositional to your mean free path, the order of mean free path by might be similar for gas molecules and electrons, but what is quite different is your velocities if you are talking about velocity of gas molecules approximately what is the order.

Student: (Refer Time: 23:49)

Velocity of gas molecules approximate order is a 10 power 2 or 10 power 3 meters per second.

Student: (Refer Time: 24:07)

10 power 10 powers 2 to 10 power 3 whereas, if you look at electrons what is the magnitude 10 power 5.

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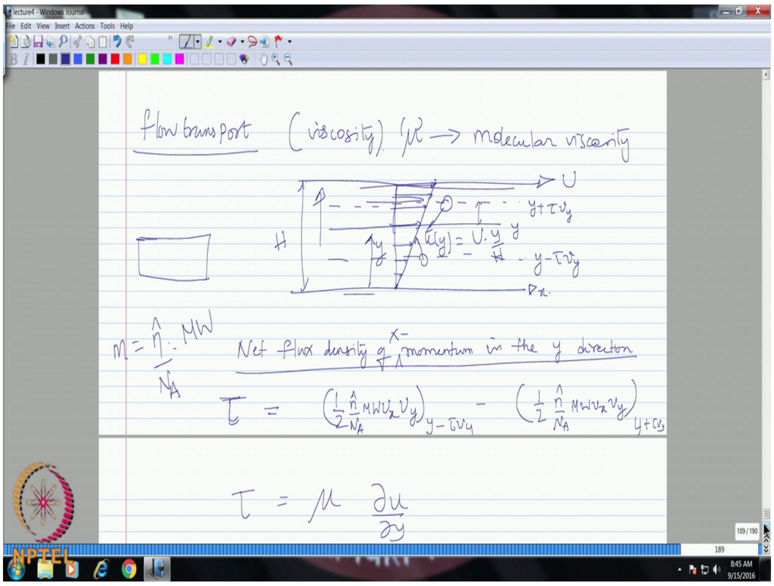

Therefore directly you can see in which case the thermal conductivity will be higher metals or gases metals correct. At a fundamental level, this is a try to the molecular velocities and relaxation time. So, similarly what we will do is, we will look at now flow transport try to derive the expression for viscosity right, now viscosity this is also called as dynamic viscosity or molecular viscosity, because of the same reason, because this is viscosity can be expressed in terms of the all the molecular characteristics. So, from the kinetic theory and therefore, this is called molecular viscosity. Now, origin is coming from inter molecular collisions.

So, if you extend this to viscosity we will take up a case of Couette flow to derive this. So, I hope many of you remember how the Couette flow is, so, you have a bottom plate which is fixed top plate, which is moving with a velocity let us say u and if you have a coordinate now the variation is primarily in the y direction, and this is an infinitely long plate. Therefore, is periodic about x you do not have to really bother about variation in the x direction here, the variation will be primarily in the vertical direction. So, if you look at coordinate system, starting from y equal to 0 to y equal to let us say h which is the separation between the plates you have a variation in the velocity profile which is linear profile, this is the characteristic of a Couette flow. So, the maximum velocity will be at the top plate u. So, to satisfy the no slip boundary condition, and at the bottom plate this is fixed. So, this will be 0 velocity and between these 2 you have a linear variation.

In fact, it will be u of y will be simply, u into y by h. So, for this case, I want to apply the kinetic theory and look at the net flux of momentum. The earlier case we looked at, net flux of energy for heat conduction now in the case of flow problem, the flow is governed by momentum gradient. So, we are looking at net flux of momentum and therefore, where we should consider the interface in which direction horizontal. So, we can draw horizontal line this could be our y for example, some y and then we can talk about some left and right boundary, top and bottom boundaries here. So, this will be y plus tau into v y right. So, this is again the distance of mean free path for the molecules before they collide and similarly at the bottom you have y minus tau v y. So, you can use the same principle to calculate your net flux density of momentum in the y direction, net flux density of momentum.

So, what does the net flux density of momentum give for a fluid element, if you draw a fluid element and stress basically. So, therefore, this net flux density will be nothing but your shear stress tau. So, I want to calculate therefore, the flux of momentum due to the molecules coming from y minus tau v y and the other from y plus tau v y you know. So, these are going crossing going up these are crossing going down. So, I want the net flux in this direction. So, this net flux is basically causing a resulting stress in this direction, because the stress is related to the gradient of the velocity. So, here we have a gradient in the vertical direction. So, that will cause a shears stress on the plate correct.

Therefore, in order to calculate this stress we have to find out, what is from the molecular picture, how this velocity gradient is now bringing in a momentum flux change. So, apply the same principle that we have done before for the energy transport and please use the Taylor series and proceed head and tell me what will be the final expression for viscosity. So, you can compare this expression with your Newton's law tau is equal to mu d u by d y in the end and then you will get an expression for mu, you can all of you do that. Now when I said net flux of net flux density of which momentum, x momentum, you have d u by d y. So, there is an x momentum, but there is a gradient in the y direction this is what you have to consider.

So, how do you write your momentum flux to be have, half of and then what is your momentum flux in general. So, if you have if you have mass of these gas molecules v into x is your momentum x momentum, momentum flux in the y direction will be m v x into v y right. So, now, what is the mass, how do you calculate it? So, now, if you look at therefore, you have n number of molecules per unit volume that is your n cap now you know the molecular weight, that molecular weight is kilogram per kilo moulds. So, you have to convert this into moulds this number density. So, therefore, what do you do divide by Avogadro's number this is gives you the number of molds per unit volume and then multiplied by the molecular weight now this will therefore, give you the mass per unit volume which is nothing, but your density.

So, therefore, the mass that we have is the mass per unit volume right. So, similarly before we define energy per unit volume, joule per meter cube into velocity gave you the flux of energy. Similarly we have the momentum x momentum the flux of this will be v y, same way this point also. So, what do you get finally, for mu?

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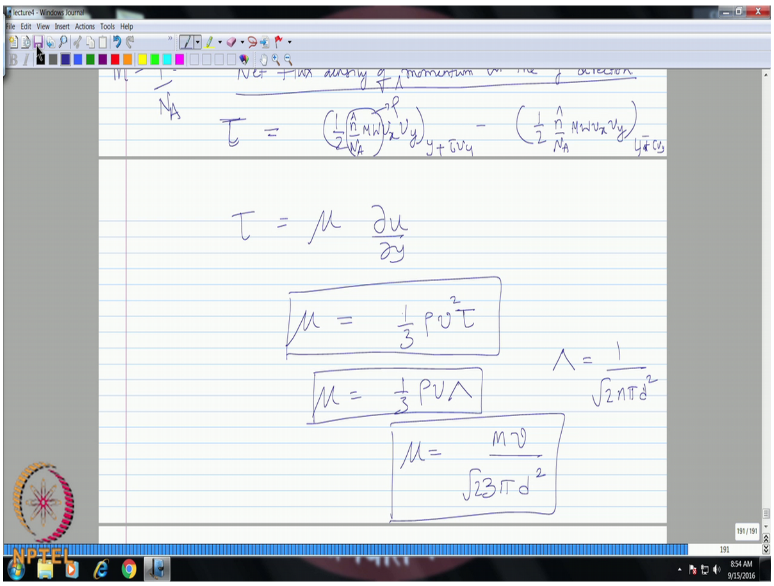

Student: (Refer Time: 40:18)

You can you can call this as density directly, this is mass per unit volume right, you can directly call this as rho and we are now looking at incompressible flows. So, therefore, rho can be assumed constant you can take out further the derivative.

Student: (Refer Time: 40:53).

So, you should be getting 1 by 3 rho into v square tau right, this is what you should be getting and if you rewrite this in terms of the mean free path. So, this will be 1 by 3 rho v into gamma. So, therefore, for the case of gases from the kinetic theory we have derive the expression for the mean free path, which is 1 by square root of 2 n pi d square right. So, that can be substituted here for gases and you will have the final expression as the mass times velocity divided by 3 pi d square. So, we have a square root of 2 also.

Student: (Refer Time: 42:44).

I think that is a negative sign coming here, but here it should not come unlike the conduction case. So, if you are looking at we have to look at the direction of the stress. So, I think this would result in stress, if you are taking the gradient in this way this should result in a stress which is like this, but if you want to look at the stress which is like this then we have to reverse this. So, then this should be y plus tau v y minus this should be then this will give you a stress which is in the positive x, that is the shear stress in the positive x direction then you will not get this negative sign because, here it is not physical to have a molecular viscosity which is negative.

So, when we derived this flux you have to be little bit careful. So, therefore, just like we derive the expression for the thermal conductivity as a function of 1 by 3 no tau c v square, we have this expression for molecular viscosity which is 1 by 3 rho v square tau. So, you know both of these therefore, so, this is function of only things we are replacing the heat capacity in thermal conductivity with now what. With what with density right in the molecular viscosity you have density appearing here, in place of heat capacity for thermal conductivity right. So, that is the one change which is making all the difference in the properties.

One is a fluid property other the other is the heat property right. So, to get this fundamental thermo physical property therefore, now you have the basic relationship between the molecular pictures in terms of mean free path velocity. So, on with these properties and when you say viscosity it is only for gases, here you have look at the picture of ideal gases for kinetic theory we cannot apply this to liquids right.

Because this says according to this your velocities will keep increasing, with increasing temperature which means that the viscosity will keep going up with temperature that is valid only for gases for liquids the opposite behavior is seen with increasing temperature viscosity drop. So, this model is not valid for liquids. So, like this you know the kinetic theory to great extent gives you the you know the expressions they may not be derived in a very you know rigorous format, but never the less very useful expressions to calculate the thermo physical properties.

So, we will kind of stop the kinetic theory, here you can use the same kinetic theory to also calculate the diffusion coefficient in the Fick's law of diffusion. So, just like you relate your heat flux to temperature gradient you can relate your mass flux to the concentration gradient and you have a mass diffusivity which can be calculated from using the Fick's law of diffusion and from kinetic theory also you can do that and therefore, you can derive a relationship between the diffusion coefficient and the molecular characteristics.

Similarly, the ohms law in electrical engineering. So, ohms law is also a relationship between the current density, which is your current flux den basically to a function of the potential gradient when you are talking about potential there. So, you have your electrostatic potential you have electrochemical potential. So, it is your voltage basically, difference that is arising from combination of these 2 mechanisms and again you can derive a relationship what is the constant in that case in the ohms law, similarly you can have electrical conductivity there. So, all these are analogues whether you talk about heat transport, momentum transport, mass transport, current transport from kinetic theory you can get some kind of reasonable approximations we will stop here.