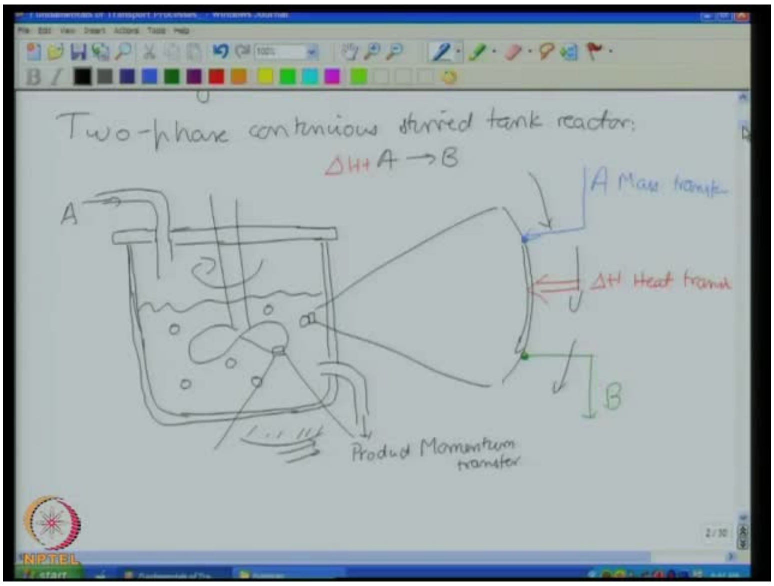
Fundamentals of Transport Processes

Prof. Kumaran
Department of Chemical Engineering
Indian Institute of Science, Bangalore

Module No. # 02
Lecture No. # 05
Dimensionless Groups Continum Description

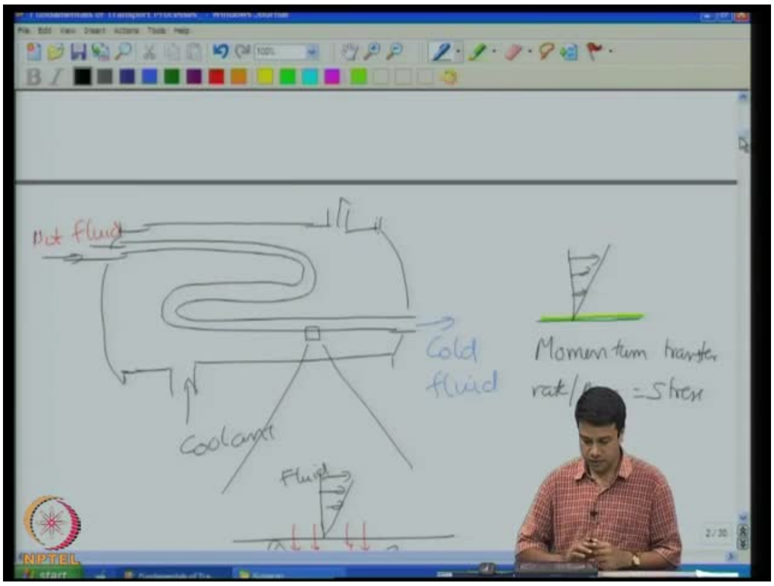
Welcome to this lecture on fundamentals of transport processes. Previous three lectures, I gave you some insight into dimensional analysis. I am sure most of you have done dimensional analysis before, but the objective of the previous two lectures was to give some physical meaning to those dimensionless groups, that we get when we do dimensional analysis.

(Refer Slide Time: 01:04)



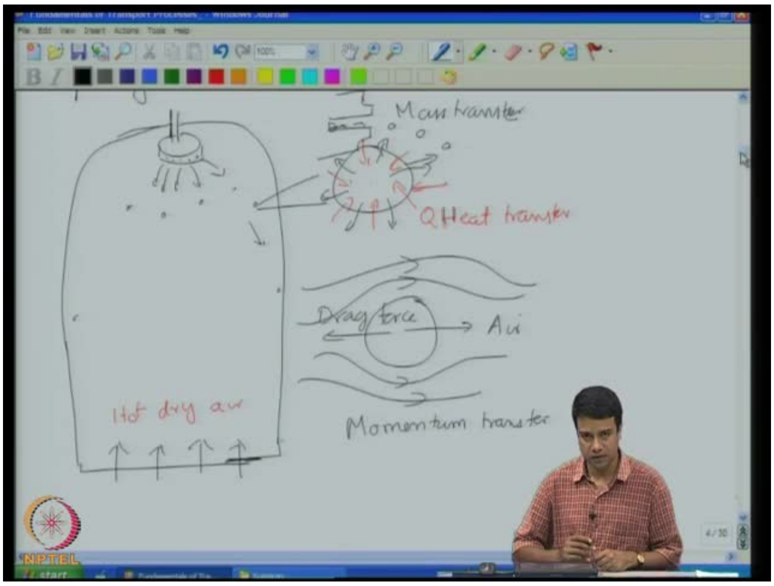
Now, it is time to turn to how we are going to analyze transport processes in this course. Previously, when we looked at the transport processes, we consider an equipment as a whole. For example, in our initial lecture on the flow through continuous reactor, we looked at the reactor as a whole and we looked at what comes in, what goes out and tried to write some balances for the fluxes that go through reactance to the surface of the reactor, fluxes of the products out and fluxes of heat either in or out.

(Refer Slide Time: 01:22)



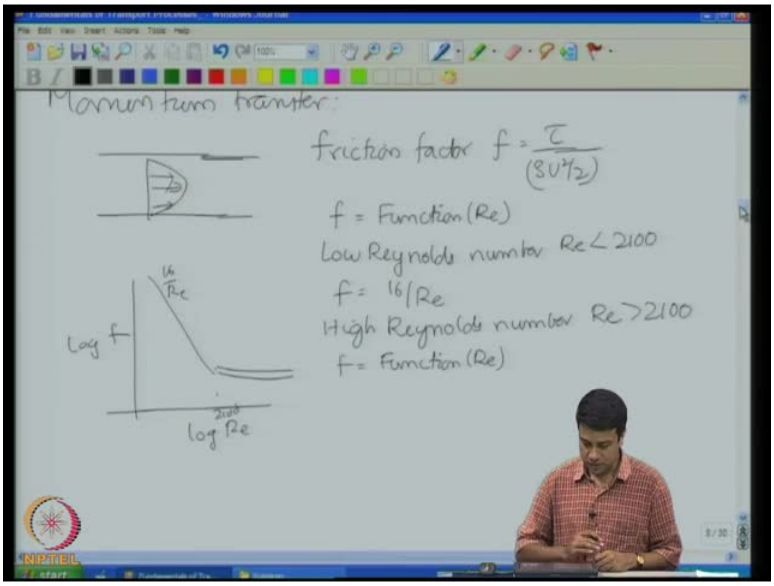
When we looked at the heat transfer problem, we were writing an equation for an average heat transfer rate and average heat flux across the entire heat exchanger, as a function of the average temperature difference between the inside and the outside.

(Refer Slide Time: 01:40)



Similarly, when we are looking at the spray drier problem, we were writing the mass flux and the heat flux, from the surface to the gas, as a function of the average difference in concentration between the particles surface and hot air, or the average temperature difference between the particles surface and the hot air.

(Refer Slide Time: 02:08)



Momentum transfer:

friction factor $f = \frac{\tau}{(\rho U^2/2)}$

f = Function(Re)

Low Reynolds number $Re < 2100$

$f = 16/Re$

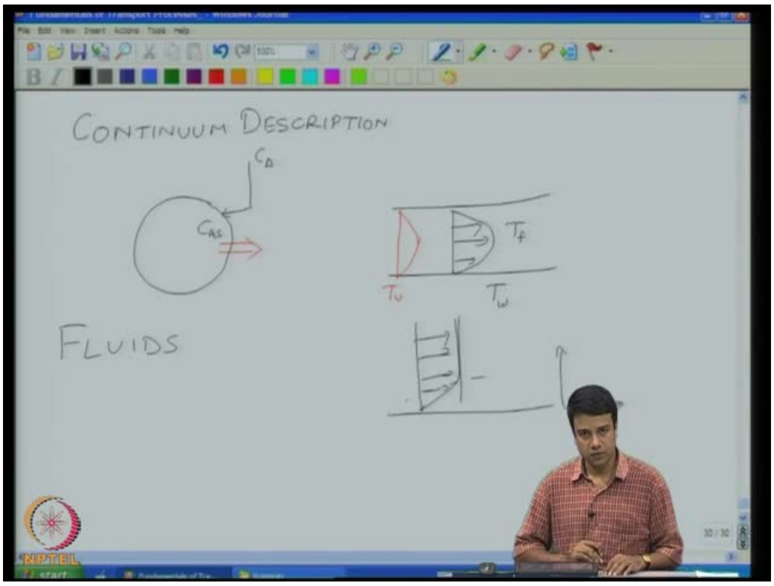
High Reynolds number $Re > 2100$

f = Function(Re)

So, in that sense, we got correlations for various situations. For example, we got correlations for the flow in a pipe, the Reynolds number; the friction factor is the function of Reynolds number and this was the average stress that is acting on the surface of the wall of the pipe, the pressure drop that is required to drive the flow. This was not the microscopic stress at every point within the flow.

So, in this course, we are going to look at microscopically what causes transport of mass momentum and energy, locally at specific locations. So, we are going to make a couple of simplifications. First thing, we are not going to analyze an entire equipment, an entire reactor, an entire heat exchange, rather we are going to focus on the location that are important for transportation process to occur.

(Refer Slide Time: 02:54)



So, for example, in the case of the catalyst pallet, we would like to find out what is the flux from the fluid to the surface. It is going to depend upon the average concentration difference between the bulk concentration and the surface concentration of the material, but the bulk concentration is not a constant. Obviously, as you come closer and closer, the bulk concentration - the concentration within the fluid - has to approach the surface concentration. In a similar manner, for the heat transfer problem, heat that is transferred either into or outside the catalyst surface is going to depend upon the difference in temperature between the surface and the bulk.

Of course, the temperature is not going to be a constant throughout the fluid. As you come nearer and nearer to the surface, if the catalyst particle is hotter, the temperature is going to be larger at the surface than in the bulk. So, how do these variations give rise to these fluxes?

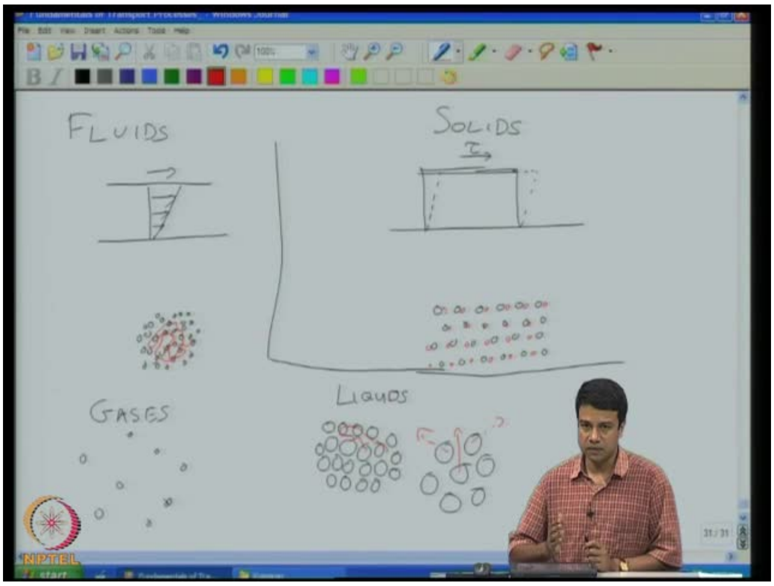
Similarly, in the case of the heat exchanger problem, we plotted the average heat transfer rate as a function of the average difference between the wall temperature and the average fluid temperature. The fluid temperature, of course, is a function of location within the heat exchanger. For example, if the fluid is hotter than the wall, then the temperature is going to be large at the center of the heat exchanger, it is going to decrease and reach the wall temperature at the wall. When you do empirical correlations, this variation is all approximated as just one constant temperature.

In this course, we want to find out what is the temperature variation itself. That involves two things. One, necessarily the configuration that we analyze will be much simpler. You will take either the flow through the tube, the flow past some flat plate, we have some velocity profile near the flat plate and we would try to find out the dependence of the temperature with height away from the surface as well as how it varies along the plate and of course, the flux can be determined from the variation of temperature near the surface using the Fourier's law for heat conduction.

Similarly, for the catalyst surface, we will try to calculate the temperature field everywhere around the catalyst surface. We will not just try to approximate it as a one constant in one location and another constant in another location, but rather we want to actually evaluate how that temperature varies as the function of location as you move closer and closer to the catalyst surface.

So, because of that our description will necessarily be simpler. We will not consider the large equipment that we have been considering before, but rather before we will just consider what happens locally at the catalyst surface, near the wall of the tube, near the wall of a flat plate and so on.

(Refer Slide Time: 06:25)



So, first things first. In this course, we will be dealing primarily with fluids. Now, materials can be classified broadly into two types. One is fluids and solids. So, mechanically the difference between a fluid and the solid is that if I take a block of a solid and I apply a stress or a force along the surface, that solid will deform for a little bit and then it will stop. So, it will deform a little and then it will stop because a solid creates a resistive force that resists the force of deformation that is applied on the solid.

If the solid were perfectly rigid, then it would not deform at all, but in general it will deform for some time and then it will stop. Of course, if you increase the stress even further, it will reach a breaking point or a yielding point, where there will be failure, but if the stress is small enough, it is going to yield for some time and then it will stop.

A fluid on the other hand, if we apply stress on a surface is going to continuously go on flowing. So, in a solid, a stress creates a deformation; it creates a displacement of solid material points around their unstressed states.

So, there is a displacement field and this displacement field can be characterized using a strain within the solid; in a fluid, an applied stress creates a velocity field; the fluid will deform continuously as long as a stress is applied and it is not going to stop until the stress is removed from the fluid.

So, solids deform and then stop; a stress causes a strain deformation in the solid. Fluids continuously deform under stresses; stress causes a strain rate in a fluid and you must be recalling the Newton’s law of viscosity which states that the stress is proportional to the strain rate; strain rate is difference in velocity divided by the distance

At the molecular level, the difference is because in a solid, all the molecules have fixed positions on a lattice. There could be different kind of lattices; there could be hexagonal close packed lattices; there could be face centered cubic lattices; there could be body centered cubic lattices and so on.

But all of these molecules, they have fixed positions and they vibrate little bit around the fixed positions, but they cannot undergo large displacements about their fixed positions. So, each atom in a solid is linked by a bond to the neighbouring atoms. The bond could be shared electron clouds in metals or other types of bonds in nonmetallic solids, but each molecule stays in its fixed location because that is at the center of attraction of all the neighbouring molecules. So, if I apply a small displacement about this location, the molecules will change a little.

The bonds between these molecules will get stretched and because of that there is a resistive force that is applied on the solid. This displacement of the molecules causes stretching which causes a force, which tends to bring the molecules back to their equilibrium locations and that effectively resists deformation.

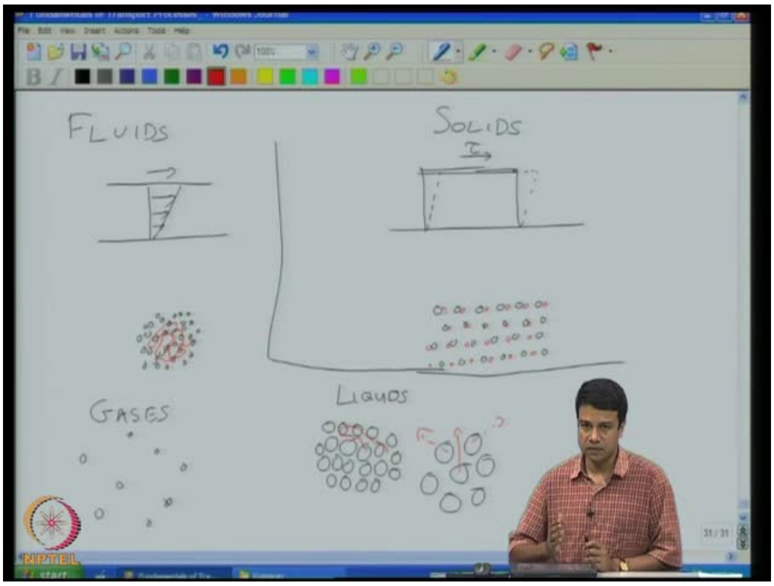
In fluids, on the other hand, the molecules do not have fixed positions. In fact, molecules in a fluid are in a state of constant thermal motion and the thermal velocity, as you would know is given by the equipartition of energy and is equal to 3kT by n. So, molecule in a fluid is undergoing some random motion; it has no fixed position, but it undergoes a random motion with time and because of that, if I apply a stress in a fluid, the molecules can rearrange themselves in such a way as to accommodate the stress that has been created and obviously, since the molecules can diffuse around, they do not have fixed locations. Therefore, if we apply a stress, the fluid will continuously deform.

Important to note: this difference has applications both for mechanical properties, the fluid deforms continuously, whereas the solid deforms and then stops but, also for diffusion. The diffusivity of these molecules in the fluid gives rise to the diffusion of mass, momentum and energy, as we shall see in the next lecture whereas, in the solid, the molecules do not diffuse apart from mechanism such as vacancy migration and interstitial diffusion, which are very slow processes.

So, this is basically the difference between the fluids and solids. In this course, we will deal primarily with fluids with the exception of heat transfer, heat conduction. Heat conduction occurs by the same Fourier’s law, whether it is in solids or in fluids.

The mechanisms are different. In fluids, heat conduction can occur because of the physical motion of molecules; in solids, it cannot. Heat occurs due to the transmission of energy by the vibrational modes of solids. However, the equations for Fourier’s law for heat conduction for both solids and fluids are the same; only the thermal conductivity, the constant in that equation changes and therefore, for heat transfer what we do will be equally applicable to solids as well as fluids.

(Refer Slide Time: 06:25)



Fluids can further be subdivided into gases and liquids. The basic difference between gases and liquids is the distance between the molecules in gases and liquids. In gases, the molecular distance is much larger than the molecular diameter. It would be typically 10 to 100 times larger than the molecular diameter.

So, in gases, the molecules actually meet through rare interaction events, which are called collisions in kinetic theory of gases. Molecules move large distances between successive interactions between neighbouring molecules and because they move large distances, the mean free path, the distance between the successive collisions is large compared to the molecular size.

In liquids, on the other hand, the distance between molecules is comparable to the molecular size. Each molecule in the liquid is sitting in or close to the potential well of attraction of the neighbouring molecules in the liquid.

Because of that the molecules are frequently in interaction with all their neighbouring molecules and they do exhibit diffusion, but however that is a slow process because for one molecule to diffuse in a liquid, it is necessary that other molecules have to move out of the way. So, for example, if one molecule has to move this way, other molecules have to move out of the way before diffusion can take place.

So, molecular diffusion is a slow process in liquids; it is a faster process in gases. In the case of gases, as we shall see, the diffusion mechanism is the same. Since the molecules are not in continuous contact with each other; transport of mass, momentum, energy has to take place due to the physical motion of the molecules themselves.

In liquids, that is not true; the molecules are very close to each other and so, you do not require the transport of molecules to have the transport of mass, momentum or energy; mass transfer of course, requires the transfer of molecules.

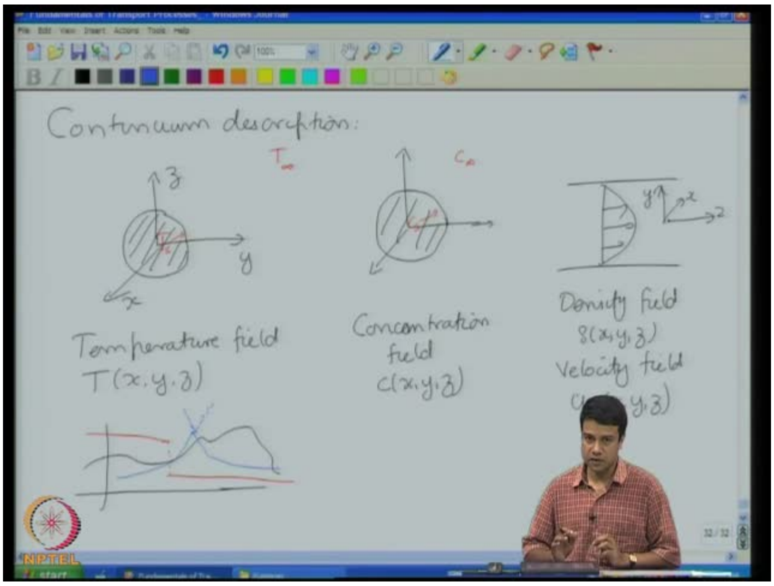
Despite the significant difference in the density between liquids and gases, because the mean free path in gases is about 10 times the molecular diameter and the mean free path in liquids or the distance between molecules in liquids is comparable to the molecular diameter, the density of gases is approximately a 1000 times less than the density of liquids. For example, water has a density of about a 1000 kilogram per meter cubed - 1 gram per centimeter. On the other hand gases, air typically has the density of about 1 kilogram per meter cubed or there about.

Despite this difference, the fundamental equations for diffusion end up being the same in both liquids and gases. In both cases, mass transfer - the flux of mass is related to the concentration gradient by the Fick’s law; in both cases, the flux of energy is related to the temperature gradient by the Fourier’s law; in both cases the stress is related to the strain rate by the Newton’s law of viscosity.

Because these laws are the same, the analysis that we carry out for liquids and gases will be the same. The laws are the same; the coefficients in those laws change. The coefficient of viscosity is going to be different for liquids and gases; coefficients of thermal conductivity will be different in liquids and gases and similarly, the coefficients of mass diffusion will be different in liquids and gases, but the relationships between the fluxes and the gradients in the densities of the quantities, which has been transported, those relations are the same and so, we will be able to treat both of these using the same relationships.

In this course, we will make no distinction between whether the substance is a liquid or a gas. The equations that we derive will be the same for both; the only difference is that the coefficients in those equations will change when one goes from a liquid to a gas.

(Refer Slide Time: 17:06)



Next, what is the description that we will use? So, I said we will analyze simple situations such as the transport around a catalyst pellet or a spherical droplet, the transfer across the surface of a pipe and other conduits across a flat plate and so on.

Let us assume that we have a catalyst pellet here and we were looking at the heat conduction problem. The surface of the catalyst pellet had a temperature T s and the temperature far away was some other temperature T infinity. Of course, as you approach closer and closer, temperature is going to go from T infinity to T s

Similarly, if we were doing mass diffusion problem, the concentration will go from C infinity to C s. So, in this course, we will use a continuum description, where we define a coordinate system, the way that I have written it, coordinate x is coming out of the screen towards you and y and z are in the plane.

So, this is the 3 dimensional coordinate system and we will define temperature field as a continuously varying function throughout the domain; so, T is a function of x, y and z.

Similarly, if you are doing a mass diffusion problem, I will have a similar situation except that at the surface, I will have some surface concentration and far away, I will have concentration C infinity, but once again I would define the concentration field C of x, y and z.

Similarly, for a momentum transfer problem, for example, if I had flow through a pipe for example, I would define a coordinate system z, x, y and here, I would define the density fields, density field as the total density mass per unit volume - rho of x, y, z and the velocity field. Velocity can be in three different directions. In this particular problem, the flow is unidirectional; I will have only one component of the velocity along the z direction. In this particular problem, the flow is unidirectional; so, I will have only one particular component of the velocity.

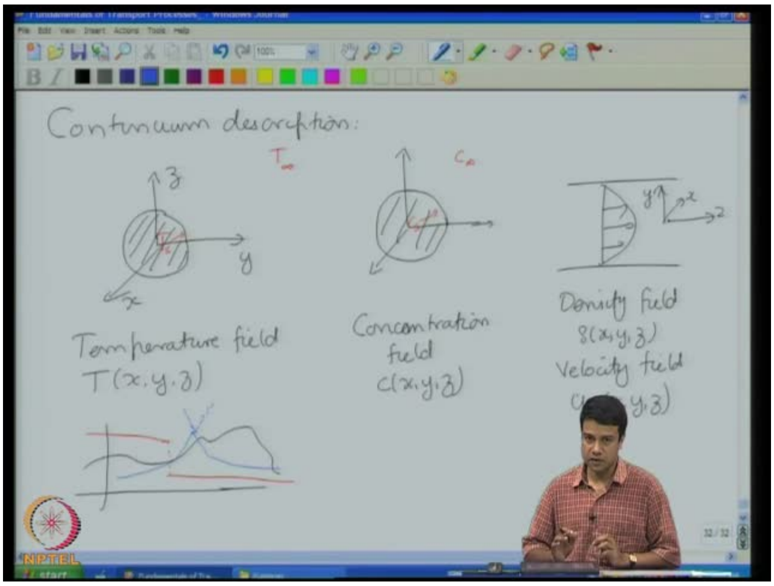
In general, you could have different components of the velocity. I have used here one component of the velocity for a particular reason. This component of the velocity is the velocity in the z direction, but it could vary with respect to both the x and y directions. So, one component of the velocity can vary with respect to all three coordinates.

So, density is a function of x, y and z and each component of the velocity is also the function of x, y and z. A function, first thing, it is a single valued function; that means that at single point in space, you can have only one value for that function temperature. So, at a fixed point in space, you can have only one value for that function. So, at a fixed point in a space, you can now have only one value for the temperature, one value for the concentration, one value for the density, one value for the velocity. So, that is the meaning of the function.

Secondly, the function has to be smooth, in the sense, that the function has to be continuous and its derivatives have to exist. So, the function that is smooth can be any function. The function that is discontinuous will have one location at which it has multiple values. There is a discontinuous transition in the value of function at one particular location.

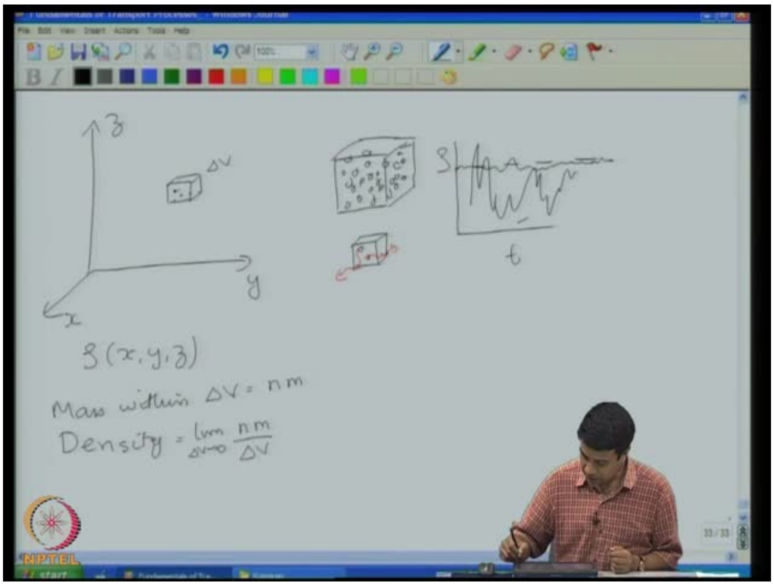
A function could be continuous, but its derivatives could have 2 values. So, for example, in the case of the blue curve, as I approach this point from the left, I get one particular slope and as I approach from the right, I get a different slope. So, the derivative is discontinuous at this point. In the present cause, all of these functions will be continuous functions and differentiable; that means, the derivatives also exist.

(Refer Slide Time: 17:06)



So, they are smooth functions, single valued functions throughout the domain. Physically, what is the meaning of this field? This function first of all is varying continuously along the x, y and z directions. So, we have a picture, where we are describing the temperature, the density, the concentration by these functions which are varying continuously in all three directions, but a real fluid has molecules in it. So, it is not just a continuous function, it actually has molecules which fluctuate about and the density within a control volume is the number of molecules in that volume divided by that volume itself.

(Refer Slide Time: 23:10)



So, how do I define the density field? At a point, if I wanted the density at location x, y, z. I construct a small volume around this point x, y and z, I construct a small volume delta V and I find out how many molecules are within this volume delta v. So, the total mass within delta V is equal to the number of molecules times the molecular mass, where n is the number of molecules and m is the mass of 1 molecule.

So, the density is defined as the number of molecule times the mass of the molecule, total mass within this volume divided by the volume delta V itself. This is for a small volume. So, this is in the limit as delta V goes to 0.

So, formally this is the definition locally of the density. So, I take one particular location x, y and z, construct a small volume around it, find out the number of molecules in that volume and as I shrink that volume, make it smaller and smaller and measure the mass within that volume divided by the volume itself. In the limit as the volume goes to 0, the number of molecules and the total mass will go to 0, the volume will go to 0, but the ratio will not go to 0, but it will go to some constant value, which is only a function of that location; it is not a function of the size of the volume in the limit as the size of that volume goes to 0.

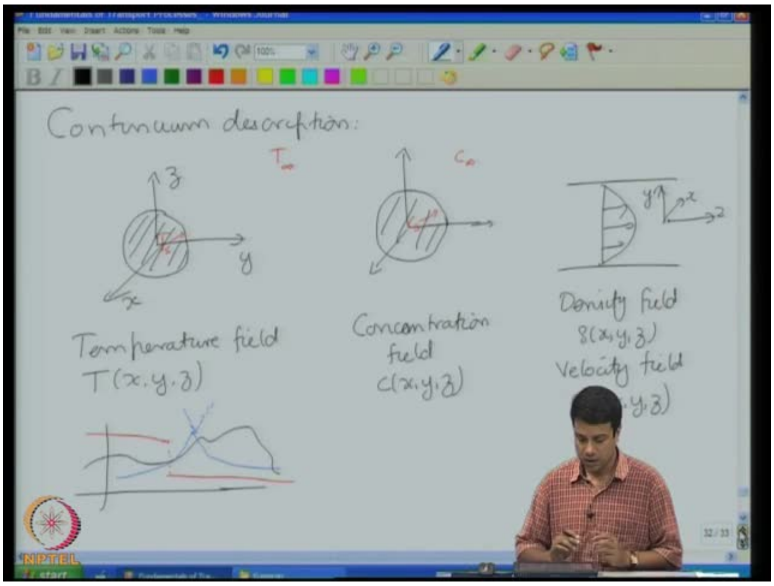
So, that is the formal definition of the density. Clearly, there is a problem with this definition. As I make my volume smaller and smaller, if I had significantly large volume, I would have many molecules in it, but as I make it smaller and smaller, I might have just a few and these molecules are in constant random motion. So, they may come into the volume or they may go out of the volume.

So, if I take this measure of density and look at the density as a function of time, it is going to undergo large fluctuations surface are that could not be negative in time when the molecule is in, we will get a large density; when a molecule is out, we will get a small density.

So, obviously, this volume cannot be as small as a molecular size or even a mean free path. When we make the system larger, you have a large number of molecules in here. So, there will still be fluctuations in the density, but they will be much smaller because when the number of molecules is large, one molecule coming in or going out; it does not make that much of a difference to the total mass of the system.

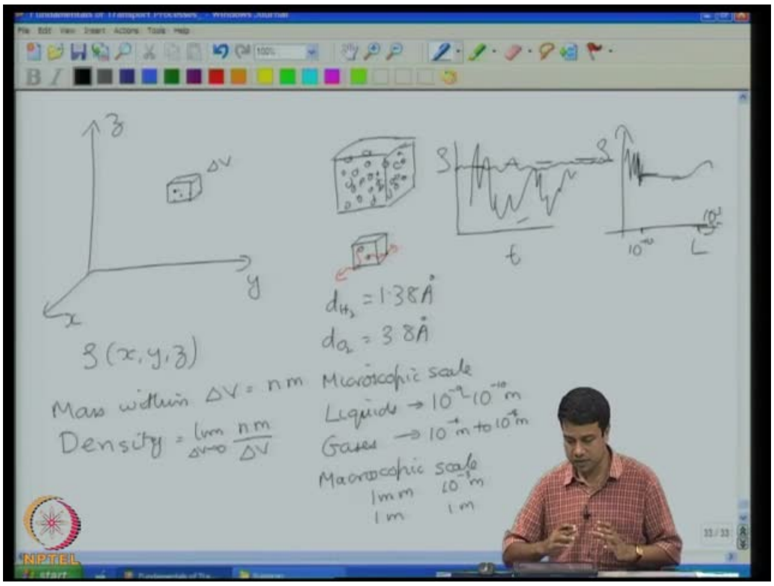
So, there will be fluctuations about some mean value, but those fluctuations will not be large. So, the size of those fluctuation decreases, as we make this volume larger and larger compared to the molecular size.

(Refer Slide Time: 27:26)



However, I cannot make this volume comparable to the catalyst particles size because I want to find out what is the variation of the concentration, where distance is comparable to the radius of the particle itself. So, the volume cannot be made too large such that it becomes comparable to the macroscopic size.

(Refer Slide Time: 28:09)



Similarly, in the case of the fluid flow, I cannot make the volume large as the tube radius itself because I want a local description. So, the volume has to be small compared to the tube radius so that I can get a local description. I can define density, concentration, temperature and so on at a given point. So, it is to be small compared to the size of the characteristic length scale of the system that we are considering. At the same time, it has to be large compared to the molecular size; otherwise, you will have large fluctuations.

So, what is the micro scale in this case the molecular size in the case of liquids or the distance between particles, the mean free path in the case of gases? In the case of liquids, we know that the diameter of let us say hydrogen molecules are approximately 1.38 angstroms; the diameter of oxygen is approximately 3.8 angstroms; the diameter of the water is about half the diameter of an oxygen molecule.

So, therefore, in the case of liquids, the size has to be large compared to this angstrom level or nanometer level molecular size. However, it has to be small as compared to the macroscopic size. So, for example, if I had a catalyst pallet of diameter 1 millimeter or a pipe of diameter 1 centimeter, the volume that I consider has to be small as compared to 1 millimeter or 2 centimeter.

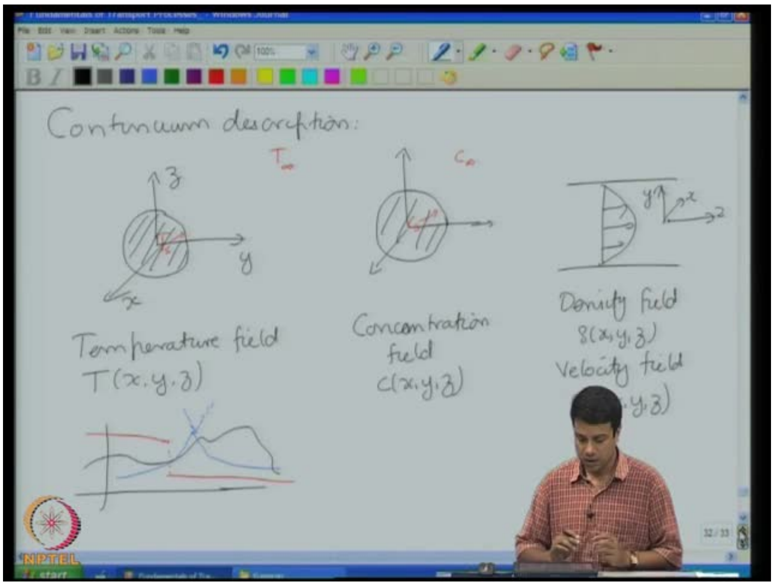
So, here I have a microscopic scale, which is for liquids; it is about 10 power minus 9 to 10 power minus 10 meters. In the case of gases, the relevant microscopic scale is the distance between molecules or the distance a molecule travels between successive interactions.

We would see a little later; we will actually calculate this in the next lecture. In the case of gases, this varies from 10 power minus 6 meters to 10 power minus 8 meters roughly 10 power minus 7, 10 power minus 6 meters. Whereas, the macroscopic scale is 1 millimeter, which is 10 power minus 3 meters to let us say, 1 meter which is 1 meter.

So, in between this microscopic scale that is 10 power minus 6 to 10 power minus 8 for gases and 10 power minus 9 to 10 power minus 10 for liquids and this microscopic scale, we have a sufficient range of scales in such a way, we can define average quantities. So, if I plot the averaging volume, the averaging length scale for the averaging as a function of density, this is about 10 power minus 10 and this is about 10 power minus 3 in meters.

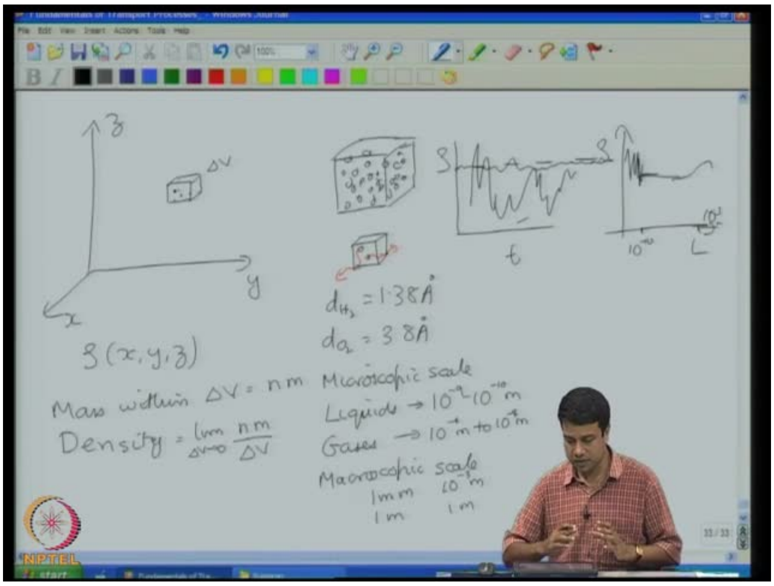
So, 10 power minus 10. I will get large fluctuations because the molecule may be inside or outside as this becomes larger, but still smaller than the microscopic scale, the density will converge to the constant value. Then, as it becomes still larger, actually, I will start getting variations again because I am actually averaging over real concentration variation within the system.

(Refer Slide Time: 27:26)



I am actually averaging over density differences across the pipe or over length scales comparable to the radius of the catalyst particle. So, this microscopic volume is defined in such a way that it is large compared to the molecular size, but still small compare to the macroscopic scales.

(Refer Slide Time: 28:09)



$\rho(x, y, z)$

Mass within $\Delta V = nm$

Density $= \lim_{\Delta V \to 0} \frac{nm}{\Delta V}$

$d_{H_2} = 1.38 \text{Å}$

$d_{O_2} = 3.8 \text{Å}$

Microscopic scale

Liquids $\to 10^{-9}$-10^{-10} m

Gases $\to 10^{-7}$ m to 10^{-8} m

Macroscopic scale

1 mm 10^{-3} m

1 m 1 m

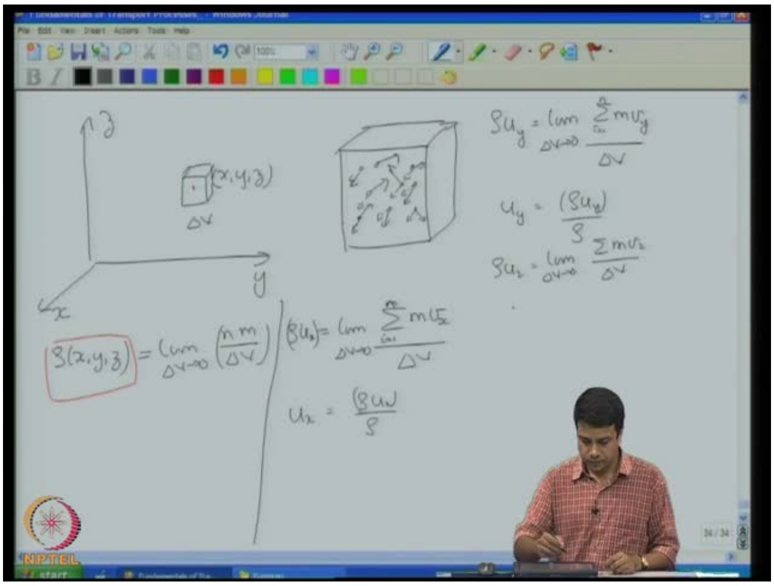
The definition of this requires that I have a sufficient range of sizes, sufficient range of length scales between the microscopic scale on the one side and the macroscopic scale on the other side such that I can find scales in between, which are large compared to molecular size or mean free path, but still small compared to the macroscopic scale; over that volume, I can do this definition of density.

So, the volume cannot be too small; it cannot become smaller than a molecule; it has to be much larger than a molecular size, but still small compared to the macroscopic scales in the problem.

If I define my volume in that range and I draw volume around a point, count the total mass within that, divide by the volume in the limit as this goes to 0 in comparison to the macroscopic scales, but still large compare to the molecular scales, I will get a constant value for the density. As I vary the size so along that it is large compared to the microscopic scale, but still large compare to the molecular scale, but still small compare to the microscopic scale, in this range, I will get a constant value. That is defined as the density at that particular location in the continuum approximation.

So, that is the physical meaning of the density field. At each location I draw volume, find the mass in that volume, divide by the volume in the limit as that volume goes to 0 compared to the microscopic scales, but is still large compared to the molecular scales, I can define a density. If my system size is very small, if my system size is comparable to the molecular scales, in nano technology applications, for example, in that case, we cannot define a continuum density and as we shall see in this course, once you can define continuum fields, then you can do some pretty complicated analysis for those continuum fields. If the molecular size is not small compared to the macroscopic length scales, you do not have that, you have to consider the system as a collection of discrete particles.

(Refer Slide Time: 34:10)



So, this is the definition of the density field. So, this is the location x, y, z and I construct a small volume around this location delta V. That is the volume delta V and then I take the limit as delta V goes to 0. So, in the limit as delta V goes to 0 of number of molecules times the mass of the molecule divided by delta V is equal to the density field.

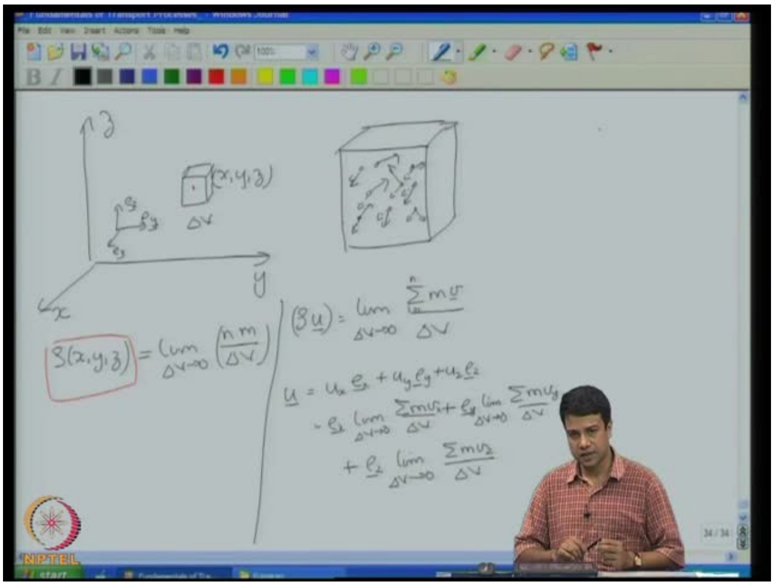
How about the velocity fields? So, let us take for example, we will take velocity in the x direction. So, in this differential volume, I have a large number of molecules and these have some fluctuating velocities to them. I can take the summation over all the molecules, i is equal to 1 to n of the molecular mass times the velocity of that molecule in the x direction.

So, I go for all the molecules. Each molecule has one particular velocity along the x coordinate; this is x coordinate coming out of the plane of the board and take the component of the velocity along the x direction, for each of these molecules. I add them all up; add up all the x components of all the molecules within this differential volume, divide by the volume and I take the limit as delta V goes to 0. This is equal to the momentum density; this is the mass times the velocity that is, the momentum value summed over all of the molecules divided by the volume. So, this is the momentum density; this is rho times the momentum density u x. So, this is the density times velocity in the x coordinate and the velocity u x is determined as rho u x divided by rho. So, the ratio of the momentum density defined in this manner over all the molecules divided by rho is the velocity.

If the molecules had purely fluctuating velocities, they have equal probability of having velocities in the plus x direction and the minus x direction. In that case, this means the velocity in the x direction will be identically equal to 0. It is only if there is the net flow that the molecules are biased towards the velocity in one direction or other. Only then, will you get a non-zero velocity u x.

Similarly, one could do this for the other components of the velocity as well. I could define rho u y is equal to the limit as delta V goes to 0 of summation i is equal to 1 to n of m times V y, where V is the molecular velocity and this divided by delta V and then we could define u y is equal to, this divided by the density; the density field I have already calculated over here. So, that is how you define the components of the mean velocity. Similarly, rho u z is equal to limit as delta V goes to 0 or summation of m V z by delta V.

(Refer Slide Time: 39:02)



$$\boxed{\rho(x,y,z)} = \lim_{\Delta V\to 0}\left(\frac{n m}{\Delta V}\right)$$

$$(\rho\underline{u}) = \lim_{\Delta V\to 0}\frac{\sum^{n} m\underline{v}}{\Delta V}$$

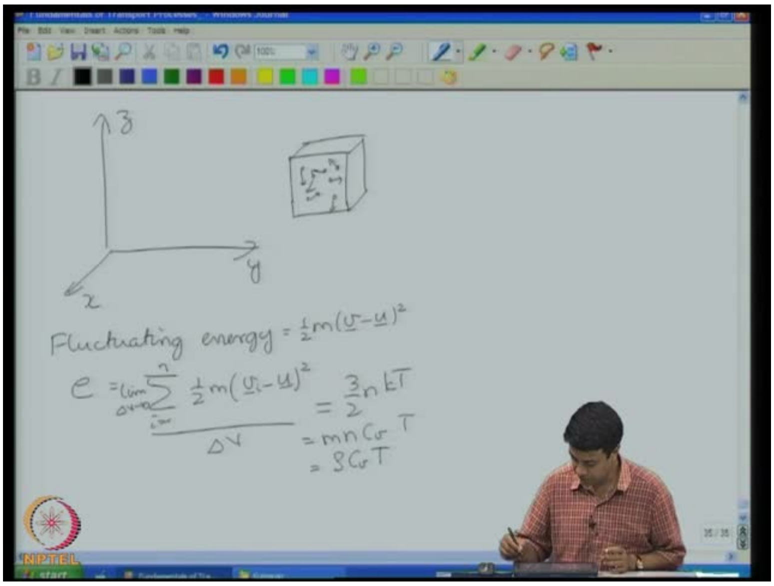
$$\underline{u} = u_x\underline{e}_x + u_y\underline{e}_y + u_z\underline{e}_z = \underline{e}_x\lim_{\Delta V\to 0}\frac{\sum m v_x}{\Delta V} + \underline{e}_y\lim_{\Delta V\to 0}\frac{\sum m v_y}{\Delta V} + \underline{e}_z\lim_{\Delta V\to 0}\frac{\sum m v_z}{\Delta V}$$

However, I do not have to think of it in this manner. I could very well define the velocity vector itself. I could define the momentum density as the density times the velocity vector itself. So, I could define a vector momentum density; u stands for a vector and is equal to limit as delta V goes to 0 of summation over all molecules of mass times the velocity vector divided by delta V, for i is equal to 1 to n.

So, this is a vector summation over the velocity vectors of each of the molecules and we will see later in the course, there are certain advantages treating this as a vector itself. Of course, if we expand this out, you will get precisely the same thing that I got earlier. So, if I define u vector is equal to u x times e x plus u y e y plus u z e z, where e x, e y, e z are the unit vectors; e x, e y, e z - these are 3 unit vectors in the 3 coordinate directions. This is going to be equal to x times the limit as delta V goes to 0 of summation of mV x by delta V plus e y times the limit plus e z and the rest of the formula as shown in the slide.

So, this will be the three components of the velocity, where u x is equal to summation of mV x by delta V, u y is equal to mV y divided by delta V and u z is equal to mV z by delta V. So, this is just an expansion, but I am just trying to point out that you could very well define the momentum vector itself. So, rho times u - this is the momentum density vector. Momentum is a vector because it has a direction associated with it. It is just the summation of the momentum of all the particles within this control volume.

(Refer Slide Time: 41:15)



Fluctuating energy $= \frac{1}{2}m(\underline{v}-\underline{u})^2$

$$e = \frac{\lim\limits_{\Delta V \to 0} \sum\limits_{i=1}^{n} \frac{1}{2}m(\underline{v}_i-\underline{u})^2}{\Delta V} = \frac{3}{2}nkT = mnC_vT = \rho C_vT$$

So, that is how you define the momentum density field. The temperature field is a little more complicated. The temperature field has to do with the fluctuating velocity of the molecules.

Now, if you had a control volume in which you had, let us say, a monatomic gas so that it had only the translational degrees of freedom. The total energy of fluctuations within this volume is calculated as follows. For a single molecule, the fluctuating energy, if it had only translational degrees of freedom could be equal to m times V minus the average velocity square; this is the kinetic energy of the voltage fluctuations alone. That is the kinetic energy associated with the mean motion and then if we subtract out the kinetic energy of mean motion, we get the kinetic energy of the velocity fluctuations.

This is the fluctuating energy of a single molecule. The fluctuating energy density is calculated by summing this over all of the molecules. Summation i is equal to 1 to n of half m into V i minus u whole square; this divided by delta V in the limit as delta V goes to 0.

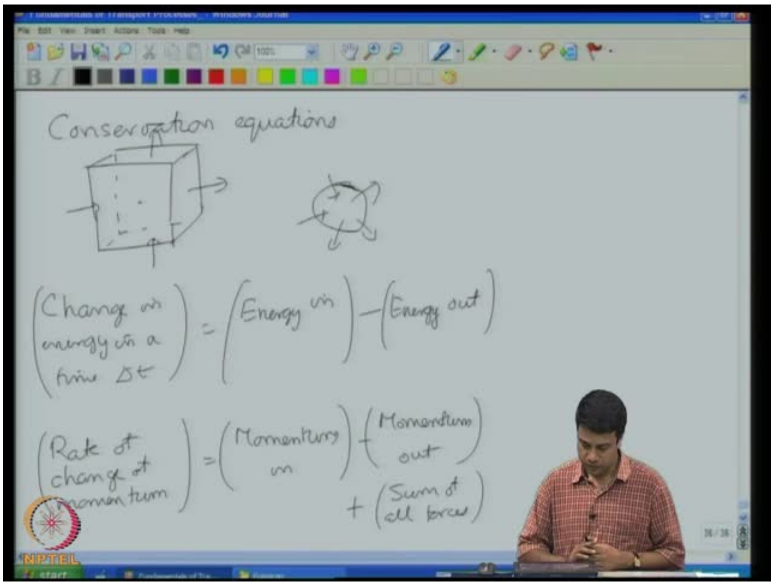
So, this is half m V r m s square by delta V in the limit as delta V goes to 0. This has got to be equal to, from the equipartition of energy, 3 by 2 nkT, where n is the number of molecules. So, this basically defines what the temperature field is. The temperature field is related to the energy fluctuations.

So, if the molecules were not just monatomic molecules, but they had rotational and vibrational degrees of freedom, those energies would have to be included here and the number of degrees of freedom. So, this will be equal to n C v kT. I am sorry, this should have been 3 by 2 kT to m, multiplied by the mass.

The mass of a molecule times the number of molecules is just the mass density. So, this is equal to rho C v T, where 3 by 2 k is the C v for the system. Let us remove the k. So, this defines the temperature field.

Now that we have defined fields which are continuously varying functions of position. How do we work with these fields? So, basically what we are trying to do is to write down conservation equations for these fields. Basic equations - conservations of mass, momentum and energy.

(Refer Slide Time: 44:57)



Conservation equations

(Change in energy in a time Δt) = (Energy in) − (Energy out)

(Rate of change of momentum) = (Momentum in) − (Momentum out) + (Sum of all forces)

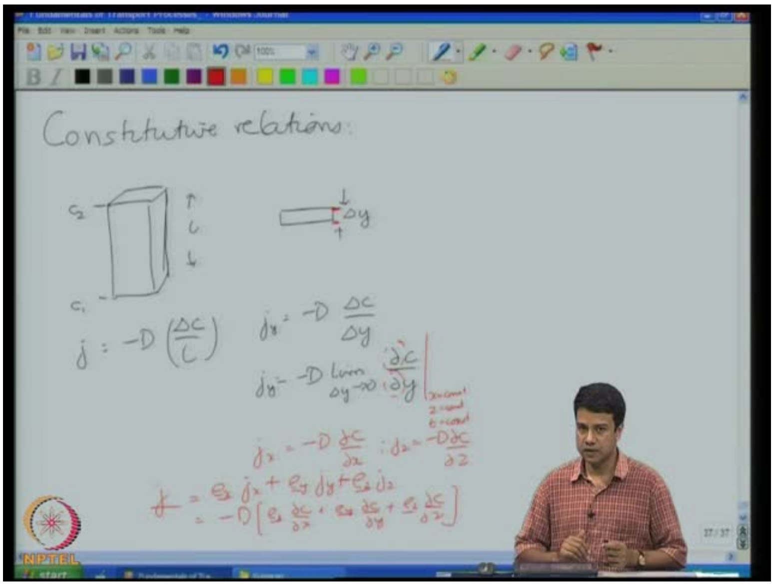
So, one component is going to be conservation equations. For example, for a differential volume, there I take locally around a point; the mass conservation will be of the following kind. Change in mass in a time delta t is equal to mass in minus mass out. So, the change in mass in a total time t is equal to the mass that comes into this differential volume minus the mass that goes out over all of the surfaces - the right, left, the front, back, in the side surfaces. You do not have to do it for a cubic volume; you can do it for any size volume. The change in mass within this volume is going to be equal to the net mass in minus the mass out of this differential volume. Exactly the same holds for energy. Change in energy is going to be equal to energy in minus energy out. The change in mass and volume is going to change the concentration locally; change in energy is going to change the temperature locally.

For momentum transfer, we use a slightly different form of the balance. It comes out of Newton’s laws of motion. Basically, what it says is the rate of change of momentum is going to be equal to momentum in minus momentum out plus sum of all forces acting on the body. So, these are the basic equations that we will use.

Now, we have defined the temperature, the concentration, the velocity at a given location and the change in momentum, energy or mass within that volume is going to determine the change in the temperature. However, the temperature, concentration, velocity are also changing with position.

So, to find out what is the energy in and energy out, we have to know how these field variables, the temperature is changing with position because as you know heat flows from higher temperature region to a lower temperature region. So, unless there is a change with position of the temperature, we are not going have a transfer of heat. Similarly, mass goes from region of higher concentration to lower concentration; unless you have the change in concentration, there is going to be no transfer of mass

(Refer Slide Time: 48:52)



Constitutive relations:

$$j = -D\left(\frac{\Delta c}{L}\right)$$

$$j_y = -D\,\frac{\Delta c}{\Delta y}$$

$$j_y = -D \lim_{\Delta y \to 0} \frac{\partial c}{\partial y}\bigg|_{\substack{x=\text{const}\\ z=\text{const}\\ t=\text{const}}}$$

$$j_x = -D\,\frac{\partial c}{\partial x}\ ;\ j_z = -D\,\frac{\partial c}{\partial z}$$

$$\begin{aligned} j &= e_x j_x + e_y j_y + e_z j_z \\ &= -D\left[e_x \frac{\partial c}{\partial x} + e_y \frac{\partial c}{\partial y} + e_z \frac{\partial c}{\partial z}\right] \end{aligned}$$

So, in order to complete the balance equation, you need to have some way of saying how the transfer - the flux of energy is related to the changes in temperature. How the flux of momentum is related to changes in velocity and how the flux of mass is related to the changes in concentration and these things are what are called constitutive relations.

We have already seen these constitutive relations. We saw for example, Fick’s law of diffusion across a surface - a slab of fluid of length L with two different concentrations. j was equal to minus D delta C by L. Similarly, Fourier’s law for heat conduction, similarly, Newton’s law for viscosity; these were written for a size of fluid.

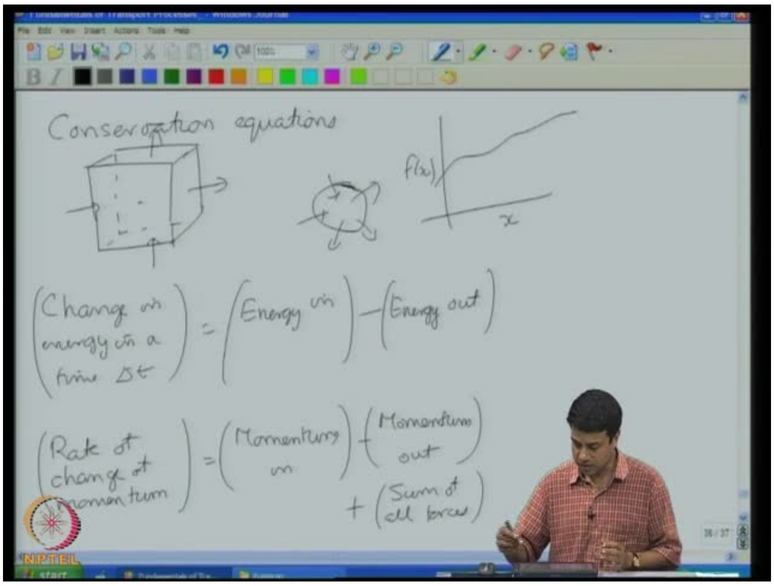
In this particular case, we would like to apply the same constitutive relations to small volumes, differential volumes in the limit as that volume goes to 0. So, these constitutive relations are to be written locally at these positions, for each differential volume.

So, if I take the same thing for a volume of infinitesimal thickness, in this direction say, delta y, j will be equal to minus D times delta C by delta y and as I make this thickness delta y smaller and smaller, in the limit as delta y goes to 0, I get dC by dy. So, this is the first derivative of the concentration with respect to the flux; this is the flux in the y direction. Note here I have used a derivative with this partial sign.

What does this mean? This means that I am taking the derivative with respect to y keeping the other coordinates are constant; x is a constant, z is a constant, time t is a constant. At a given time, I go from location y to location y plus delta y keeping x and z as a constant, find the variation C as I move. That difference divided by delta y is the partial derivative that implies that x is equal to constant; z is equal to constant and t is equal to constant. So, this is the flux in the y direction.

Similarly, I could define a flux in the x direction, minus D partial C by partial x and in the z direction. What about if I had variations in all three directions simultaneously? In that case, I will get a flux vector, which is equal to e x times j x; this is equal to minus D into e x dC by dx plus dy.

(Refer Slide Time: 52:44)



Conservation equations

(Change in energy in a time Δt) = (Energy in) − (Energy out)

(Rate of change of momentum) = (Momentum in) − (Momentum out) + (Sum of all forces)

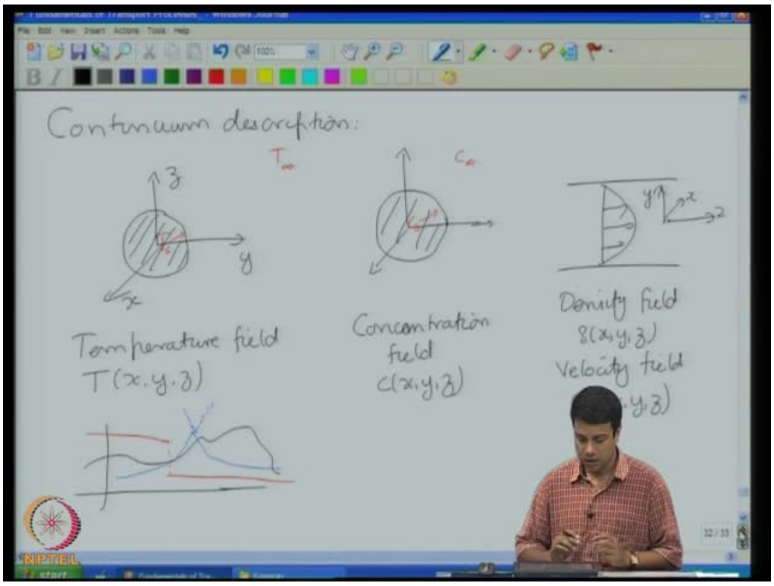
So, the point of time to get is that in this particular case, since we are dealing with all three directions simultaneously, we will get the partial derivative in the equations of motions and those equations of motion will therefore, become partial differential equations. So, locally we will do a balance at a given point in the equipment and get a partial differential equation, which tells us how the variation in temperature at that point is related to its gradients and so on, around the point from a conservation condition as well as from the constitutive relations.

So, this gives us the variation at a point. Now, we have to find the variations over the entire system and that is a process of integration. For example, if I had a curve in just one dimension, f of x as a function of x.

The derivative at a point gives me only the variation of this function at that particular location. If I want the change in function across a distance x, I have to take the derivative and integrate that over that 2 intervals.

So, there are two processes here. One is formulating the conservation and the constitutive relations themselves which lead to partial differential equations and the other is using that to solve the problem. So, these partial differential equations we will use in conjunction with what are called boundary conditions, in order to solve the problem.

(Refer Slide Time: 27:26)



So, the boundary conditions basically will tell us what is the concentration on the surface, what is the concentration far away, what is the density and velocity at the wall of the tube and what is the pressure difference across the two ends. So, those conservative equations together with constitutive relations which give us partial differential equations with boundary conditions will be solved to get the variations across the entire system.

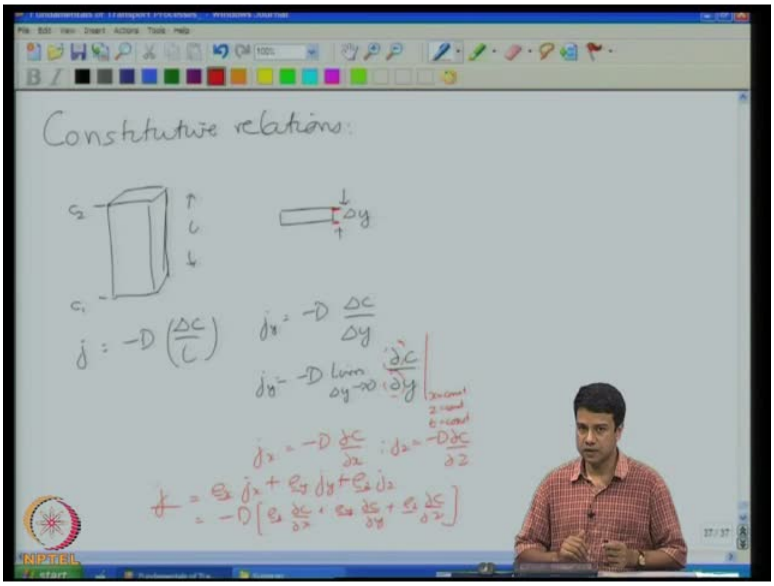
In the case of linear ordinary differential equations, there is a simple way to solve it. You are guaranteed there is a solution and that is unique. In the case of partial differential equations, there are no recipes, no algorithmic ways of solving them.

Solution of these is coupled with the physical understanding of the system. What we will do is we will look at various different regimes. One is where diffusion is dominant; the other where the convection is dominant, try to simplify the problem to the extent possible and try to get a solution, which captures the sense of the physical process that are going on without trying to be exact or accurate.

These partial differential equations can also be used in computers to get complete solutions, but that is not our objective here. The formulation as well as the physical insight which will tell us physically how solutions change as different effects which balance each other become larger or smaller. How balancing these effects is related to the terms in the differential equations; that will be the objective of the present course.

So, basically I would like to tell you the physical connection between the equation themselves and the physical processes that are going on in the real systems. Next lecture, I will start of on diffusion. This is important because as I said there are two mechanisms; one is convection and one is diffusion.

(Refer Slide Time: 48:52)


Constitutive relations:

$j = -D\left(\frac{\Delta c}{L}\right)$

$j_y = -D\frac{\Delta c}{\Delta y}$

$j_y = -D\lim_{\Delta y \to 0}\frac{\partial c}{\partial y}\Big|_{\substack{x=\text{const}\\ z=\text{const}\\ t=\text{const}}}$

$j_x = -D\frac{\partial c}{\partial x}$; $j_z = -D\frac{\partial c}{\partial z}$

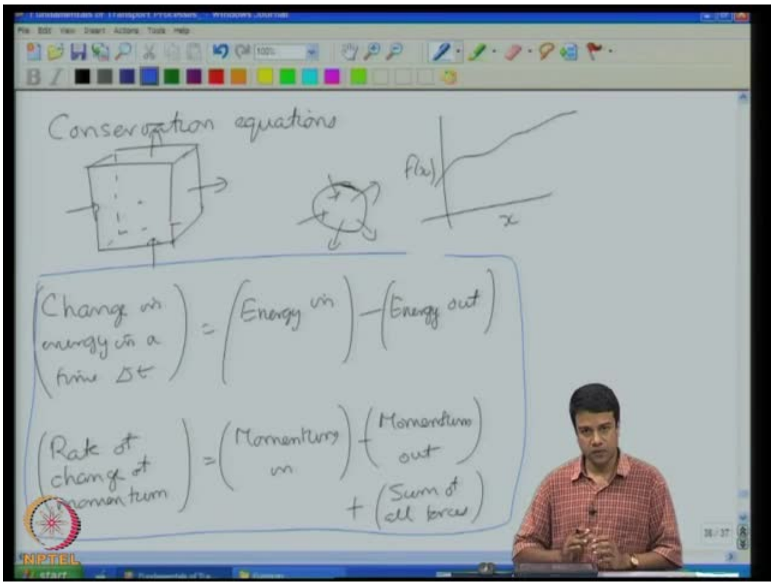
$\mathbf{j} = e_x j_x + e_y j_y + e_z j_z$
$= -D\left[e_x\frac{\partial c}{\partial x} + e_y\frac{\partial c}{\partial y} + e_z\frac{\partial c}{\partial z}\right]$

Convection is just transport to the mean flow. Diffusion is what gives us the constitutive relations, which tell us how the fluxes vary with changes in concentration and so on.

These kinds of relations are diffusion relation. They tell us how various fields vary as you change various quantities.

Next lecture, we will get a physical understanding of what is exactly the meaning of diffusion. Why diffusion happens? Can I estimate what those diffusion coefficients are just from simple physical arguments? This will give us a deeper physical understanding of the diffusion processes itself both in liquids and gases.

(Refer Slide Time: 52:44)



Conservation equations

(Change in energy in a time Δt) = (Energy in) − (Energy out)

(Rate of change of momentum) = (Momentum in) − (Momentum out) + (Sum of all forces)

Once we have done that, then we will use these balance conditions, the balance of both mass, momentum and energy in order to find out equations for variations in one direction and then to solve them for those variations in that one direction. So, we will start on diffusion in the next class and we will go on to solving real problems after we get a brief overview of diffusion and the physical mechanisms there in. So, we will see you next time.