Transport Phenomena in Biological Systems

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Lecture-78
Course Review-Part 1

Welcome, in the next few lectures, this lecture and then probably one or two more, we would review the entire course, this is a heavy course and therefore we are going to take a time reviewing it, you would be able to look at things and perspective, you would be able to revise the concepts, cement some of those concepts that are still eluding you and so on and so forth. So, that your overall preparation becomes that much better.

So it is nice to have all the review in one later on. If you want to refer to this course you can start with the review. There you have everything in a form that is there you have already gone through the effort in arriving at these various things. And based on your need, you can go to the specific lectures which are much more detailed okay.

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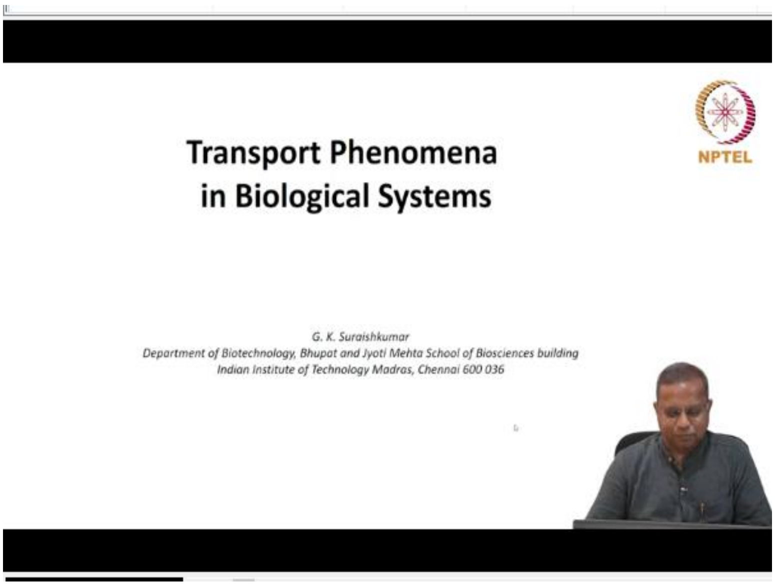

So, let us begin with the place where we began. I told you initially where this course fits in because you need to understand that to appreciate the course, a little better.

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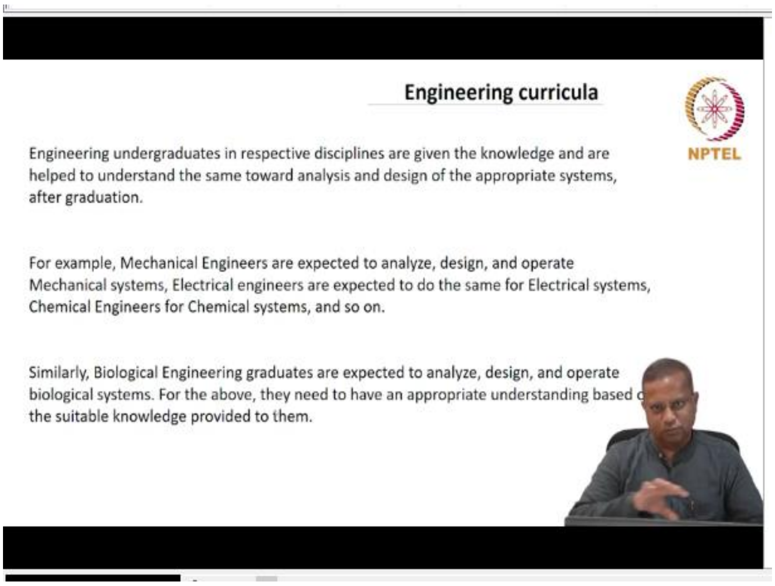

So, we looked at engineering curricula in general and we said that engineers are expected to analyze design and operate appropriate systems. Mechanical Engineers are expected to analyze and design and operate mechanical systems. Electrical engineers are expected to do the same for electrical systems, chemical engineers are chemical systems and so on and so forth. Similarly, biological engineering graduates are expected to analyze design and operate biological systems.

That is what engineering is all about. For the above they need to have an appropriate understanding based on these suitable knowledge that is provided to them was what the bottom line was.

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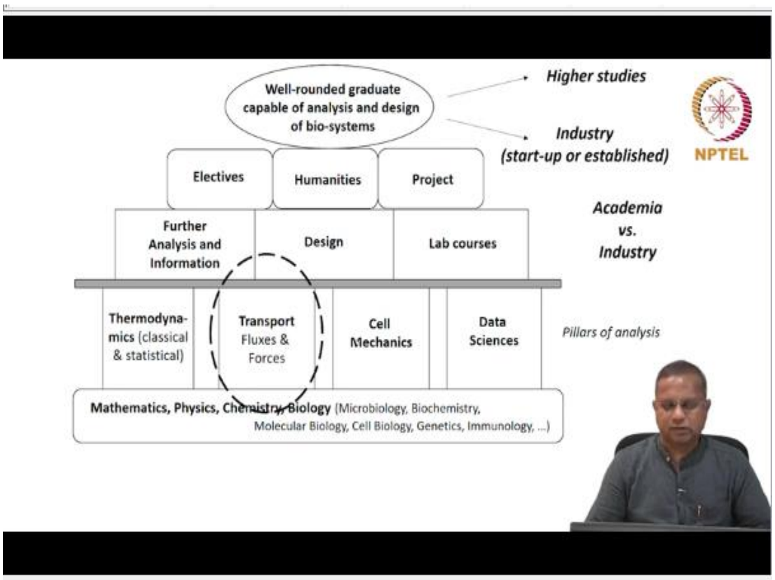

So, the curriculum is typically set up like this we have a base in mathematics, physics, chemistry and biology. We provide the base predominantly for biology, even the initial information that many students will not have. Mathematics, physics and chemistry they come in with some preparation and then that level is raised through the first year engineering courses.

And first year maths, physics, chemistry courses in engineering, then you have pillars of analysis, one of the important pillars is thermodynamics both the classical and statistical aspects for biological systems. Transport, this course fluxes and forces, cell mechanics, the courses that give you a course that looks at the mechanical aspects of cells and data sciences, the way of looking at large data sets to make appropriate sense.

All these are pillars of analysis of the basic information that is provided. So, there are courses for all these aspects and on top of this we have courses. So, further analysis as well as information, specific information, design, lab courses, which helps students develop a lot of necessary skills. Then you have electives which could be short term electives are topical or could be topical.

There is a certain interest in a certain topic at a certain time in the world. So, there is a course that is given on that mostly information and some analysis and so on. They could also be courses that built on these, which are electives. Electives this means the person has a choice to do them, which are not the essential aspects of the curriculum, but build on to the curriculum, add on to the value of the person.

Then, of course, you need humanities courses for a well rounded development of the graduate, you typically have a project to all these together, go towards making a well rounded graduate, capable of analysis and design of biosystems. Then the graduate either goes, I mean goes out into the real world and either into the industry, either a start up or an established industry, or goes for higher studies that will lead to academia or a industry.

This is the place for this course. And therefore, the importance, it is one of the pillars of analysis, important foundation for the entire curriculum and therefore it is important. We have already seen this.

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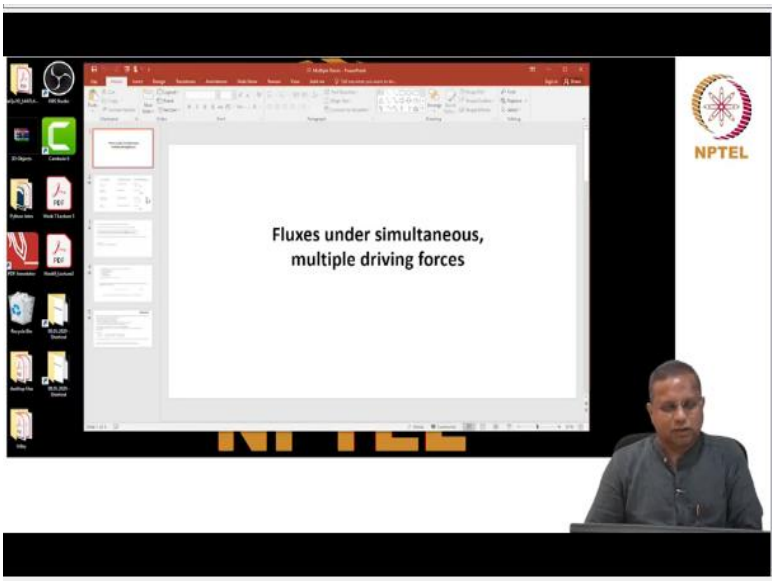

And then this is a textbook and so on, so forth. I think that is good enough for the introductory aspect of this course.

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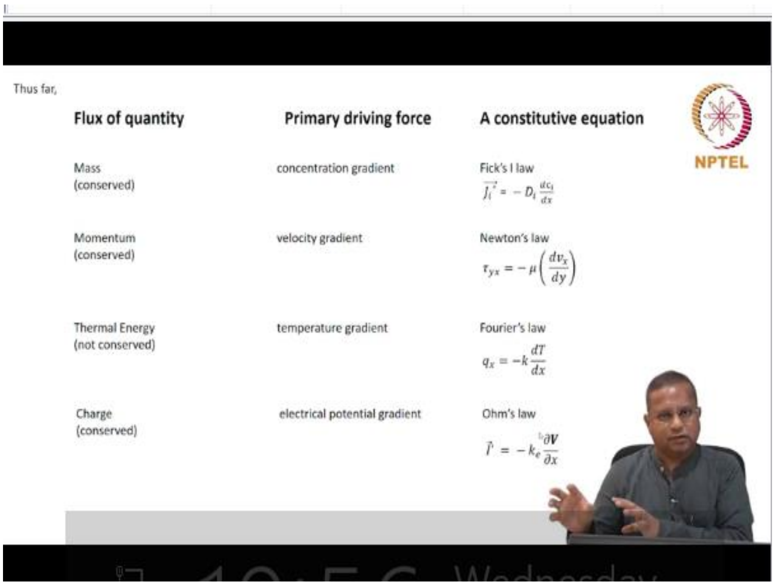

Now, let me switch to this aspect which in a nutshell puts the various perspectives together, okay. If you look at, we had essentially looked at the fluxes of conserved quantities which has mass, momentum, energy and charge okay. These are the 4 conserved quantities that we looked at in this course. If you look at the flux of that particular conserved quantity, the primary driving force for that quantity in this column.

And a constitutive equation, which is obeyed by a wide variety of substances may not be all but a wide variety of substances here, then, if you look at mass which is conserved, the concentration gradient is the primary driving force and Fick's first law gives you an example of a constitutive equation. The molar flux is directly proportional to the negative of the concentration gradient and the constant of proportionality is a diffuser.

Then if you look at momentum flux, momentum is also conserved. Velocity gradient is the primary driving force and Newton's law of viscosity, which is τ_{yx}, the shear stress τ_{yx} equals -μ$\frac{dv_x}{dy}$. The momentum flux is proportional to the velocity gradient, the negative of the velocity gradient and the constant of proportionality is your viscosity. Then we looked at thermal energy which is not conserved.

We looked at energy conservation as a whole then we kind of picked out or backed out thermal energy from this because thermal energy is of importance to us in design an operation. Temperature gradient is the primary driving force in this case and Fourier's law q_x, heat flux is directly proportional to the negative of the temperature gradient with the constant of proportionality being the heat conductivity.

You see all these forms being the same, all these ideas being the same and so on. One more charge which is of course a conserved quantity, the primary driving force is the electrical potential gradient and the Ohm's law, which is sorry the electrical charge flux being proportional to the negative of the electrical potential gradient and the constant of proportionality being the electrical conductivity k_e.

The potential gradient divided by 1 by k_e which is the resistance is your current and so on so forth. This is of course is flux, this is written in terms of fluxes to be consistent with our other representations and in this course. This gives you in a nutshell, what are we looked at in a majority of the course, where we looked only at the primary driving force causing the appropriate books. And then the last chapter was something else. Now let me go back to details. In this lecture, I look at the details of mass conservation.

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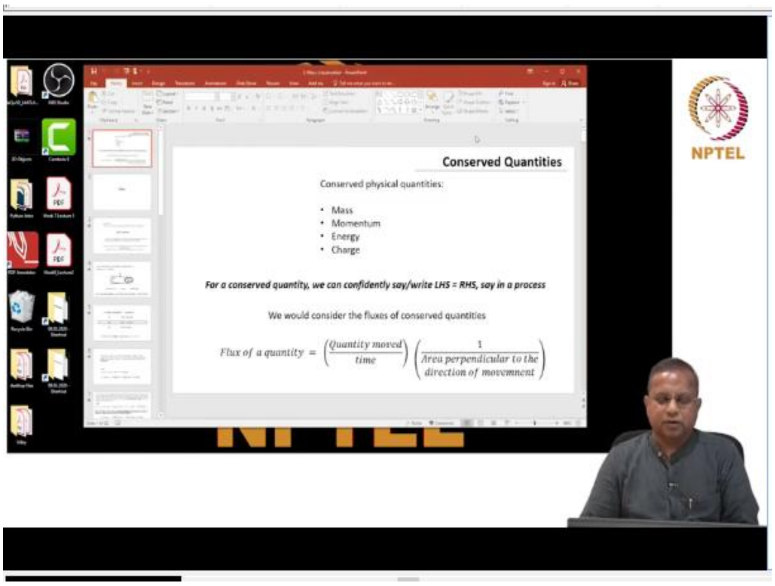

And mass flux is mass conservation is an important principle.

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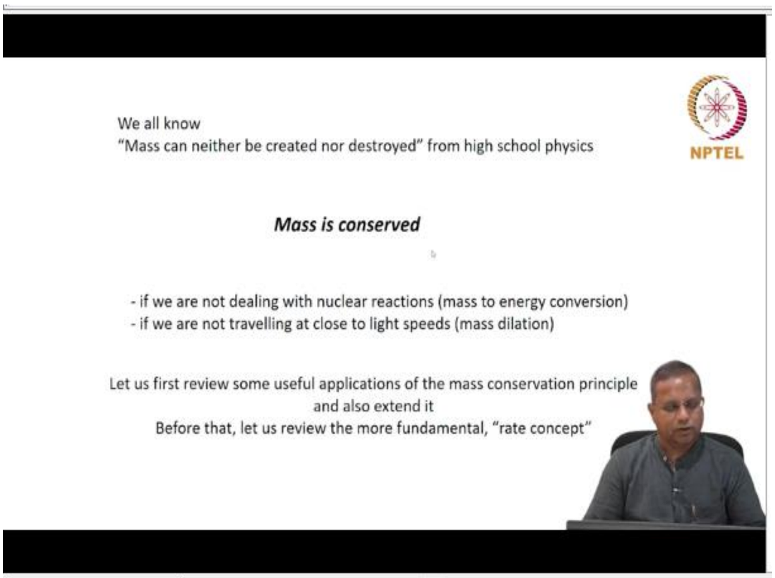

We saw the need for rates. That is where we began actually at the very, very beginning. When because engineering quantities look at rates, okay. And so we needed to write or we needed to express the mass conservation principle, mass can neither be created nor destroyed in terms of rates relevant to a process and that is the way it was going to become useful. Also, I need to mention that of course, mass is conserved as long as we are not dealing with nuclear reactions, where mass to energy conversion can take place.

Or we are not travelling at speeds close to that applied in these conditions. When you travel at speeds close to that of light, you get mass dilation. So we are not looking at that affects in the mass conservation. So, as long as you do not get into these masses conserved for all terrestrial aspects except for nuclear reactions and then they should be fine.

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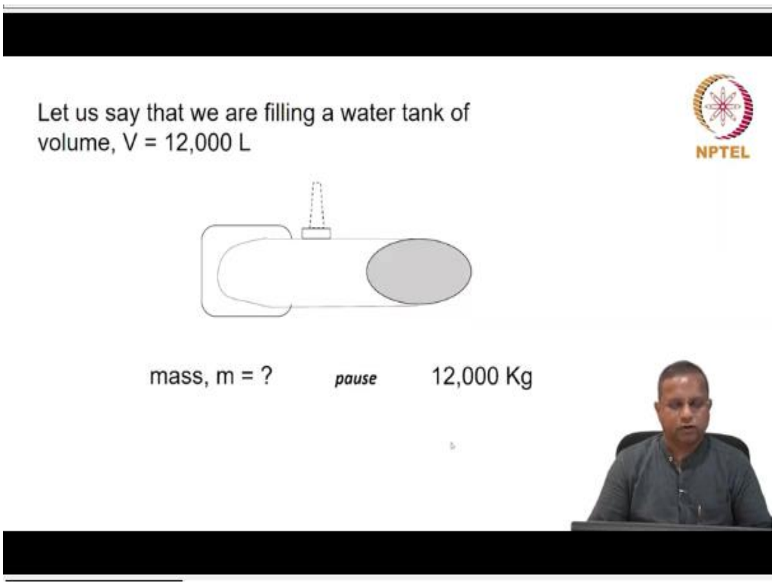

So, we had reviewed the mass conservation principle.

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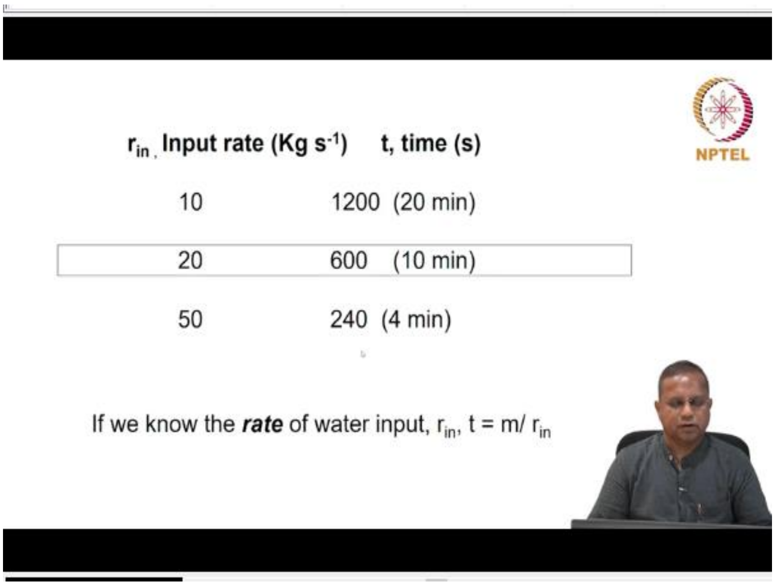

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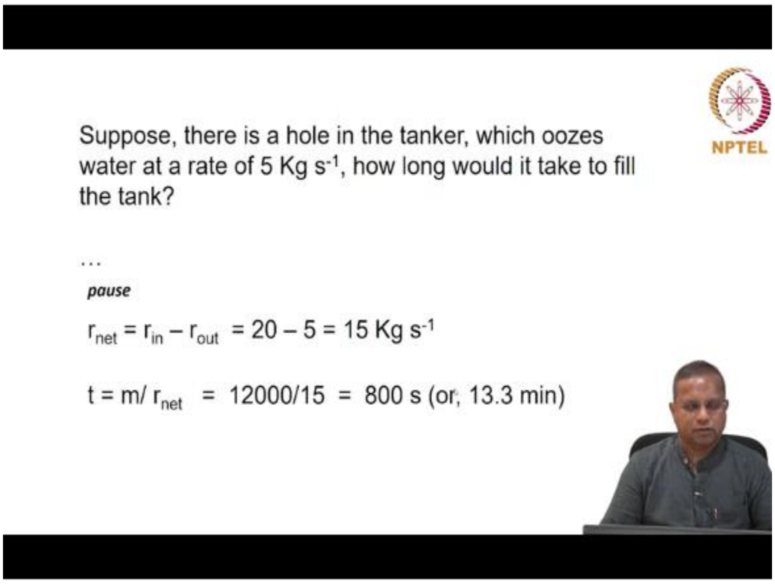

We looked at the need for it and so on.

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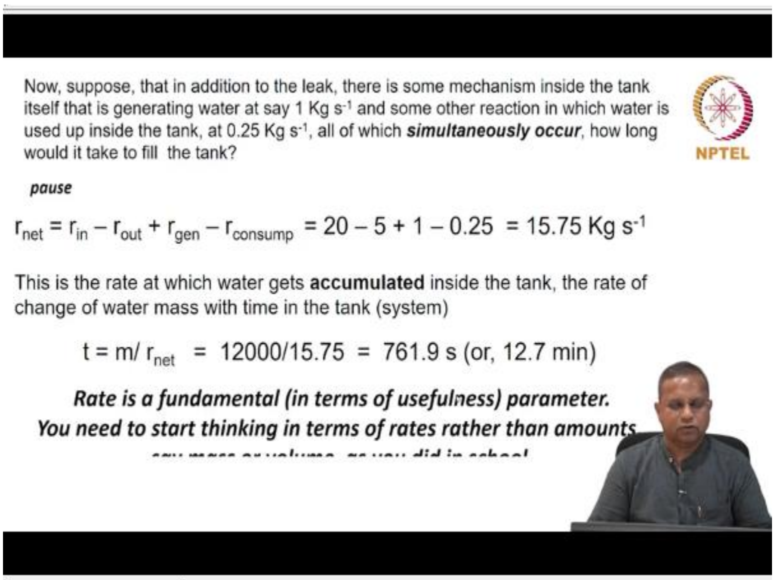

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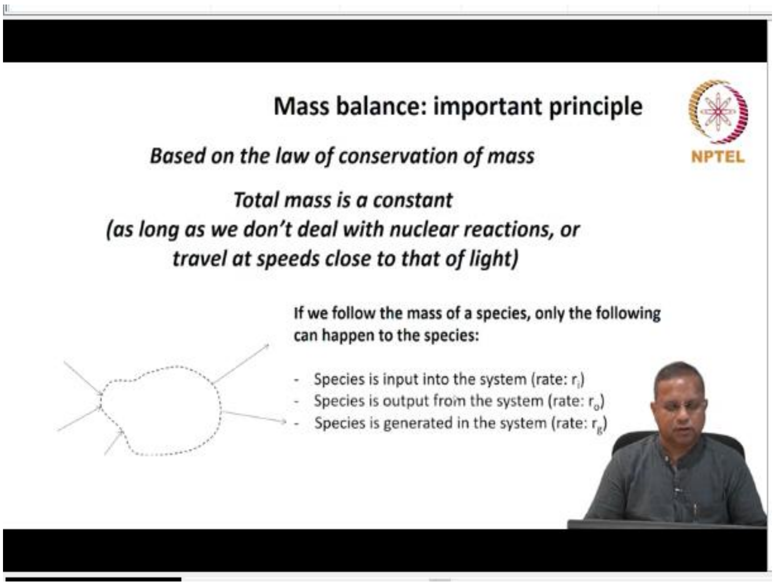

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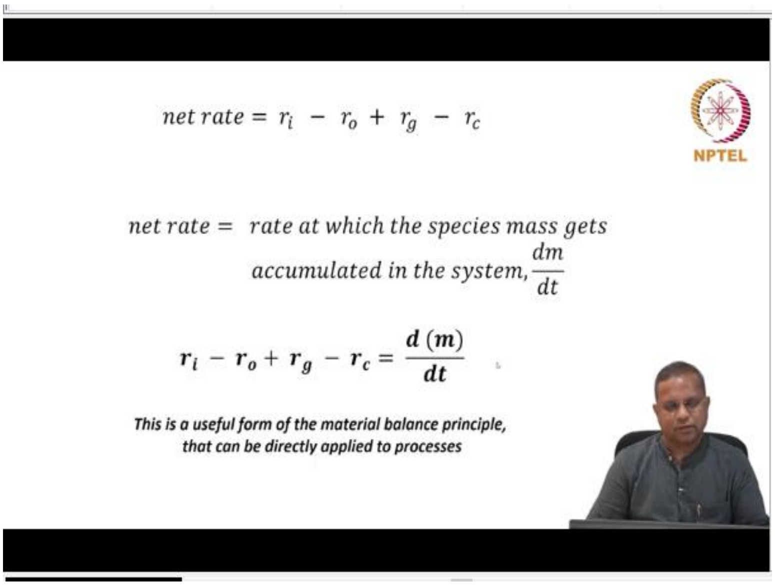

And then we got a useful form of the mass conservation equation, input rate in a mass rate minus the output rate plus the generation rate minus the consumption rate equals the accumulation rate okay. This in fact can generally be used for any conserved quantity, here we had use it for mass, then we use it for momentum, then we use it for charge and then we use it for energy and then for charge, okay.

So, this is general common sense there is nothing else than that can happen to any species. There can be when you focus on a system and you focus on a species in the system you do a balances over the system, there can be only an input rate and output rate a generation rate and a consumption rate and the algebraic sum of those leads to the accumulation rate. It is written in this form to be directly in a useful form for the various analyses.

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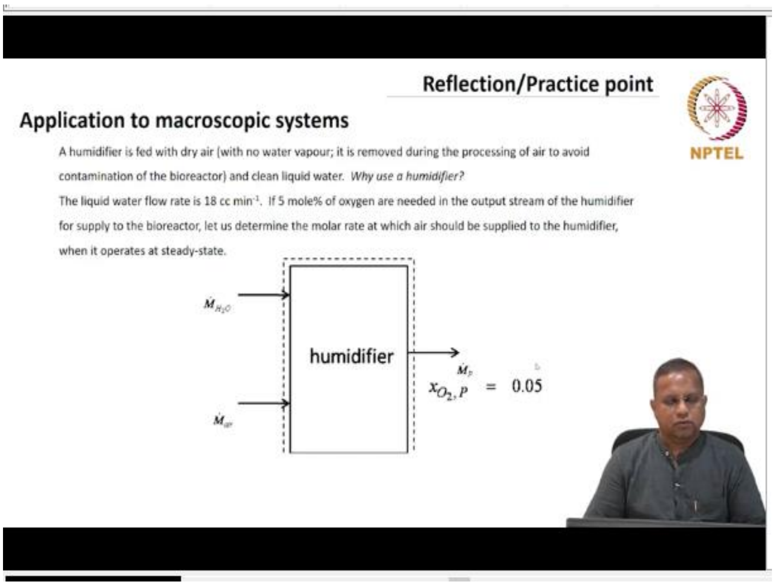

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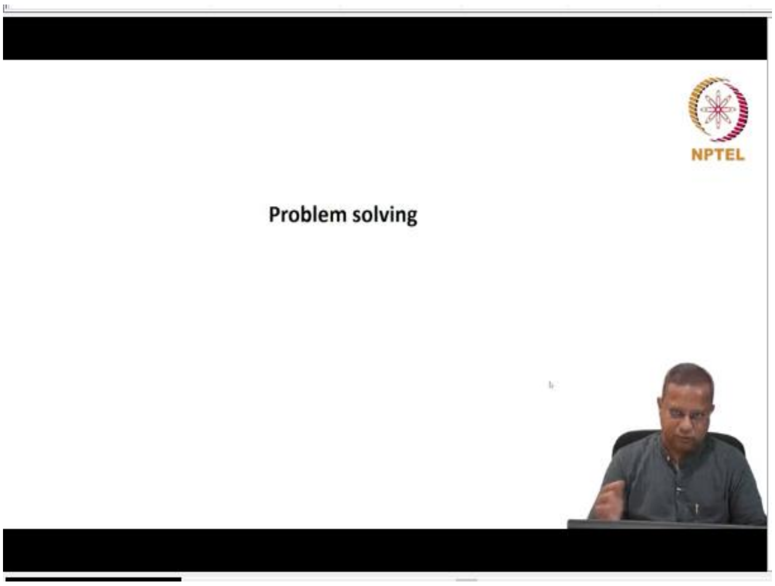

So, we had looked at the application to macro system which is a review.

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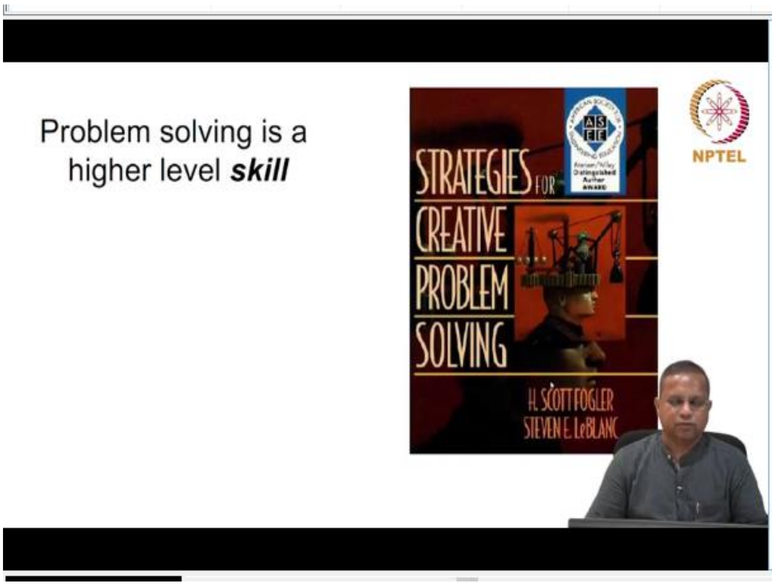

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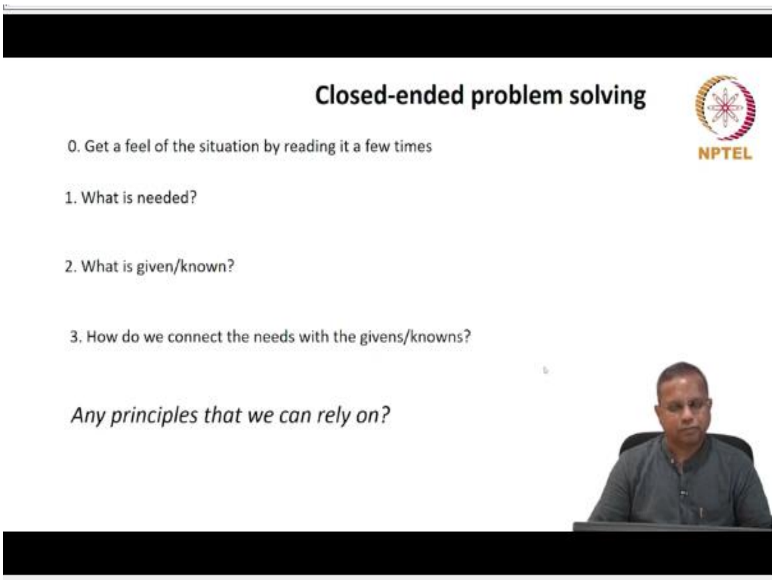

Then we looked at some principles of problem solving okay. Essentially I get a feel for the situation by reading it a few times. This is for close ended problem solving that is and then ask the question what is needed, what is given or known you could do that in any order, and then, how to connect the needs with the givens or knowns. This in general is the algorithm for getting or solving problems which are closed ended.

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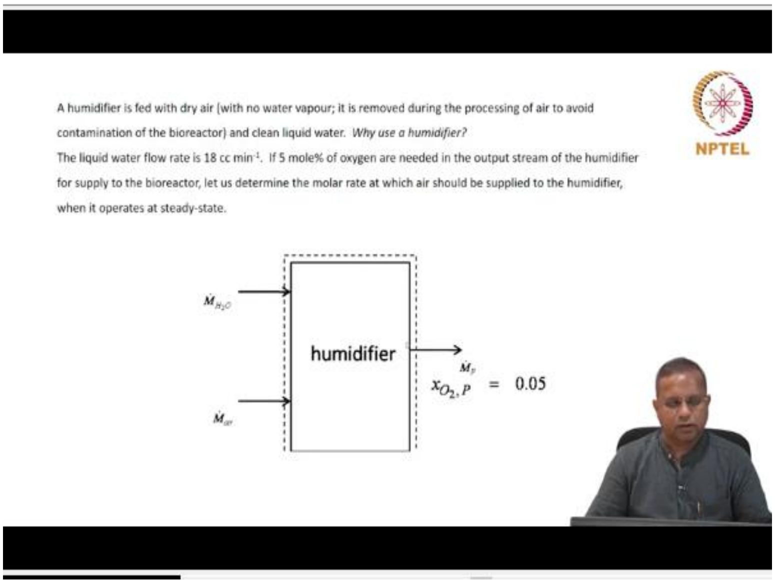

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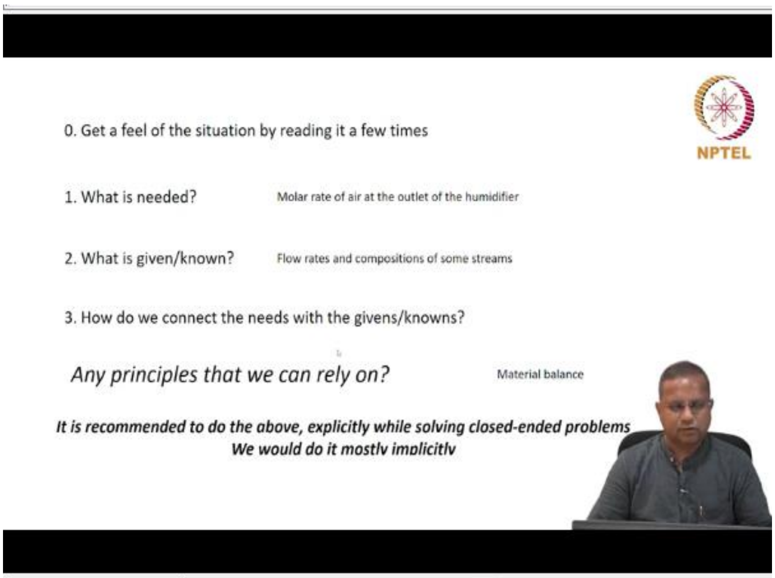

So, this was the application to a macroscopic system, which was a review.

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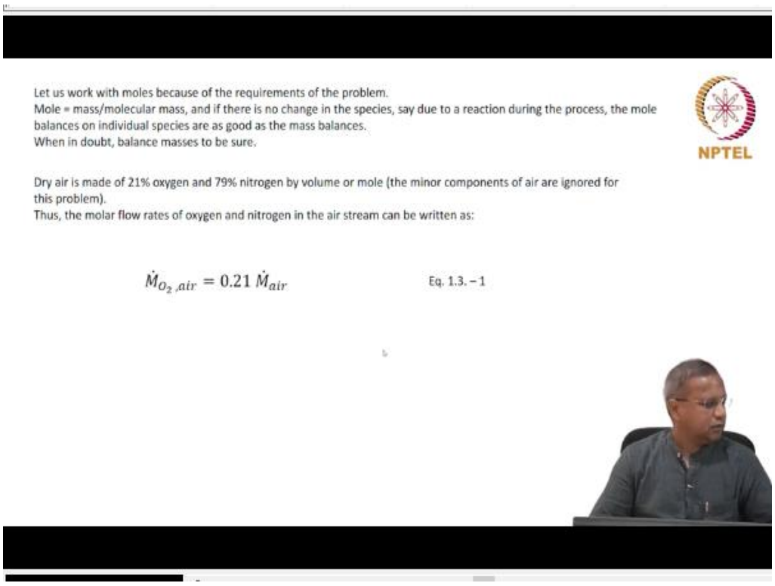

And then we applied it to a microscopic system. Maybe not spend too much here, the microscopic system, I think is here or here. Yeah, it is here.

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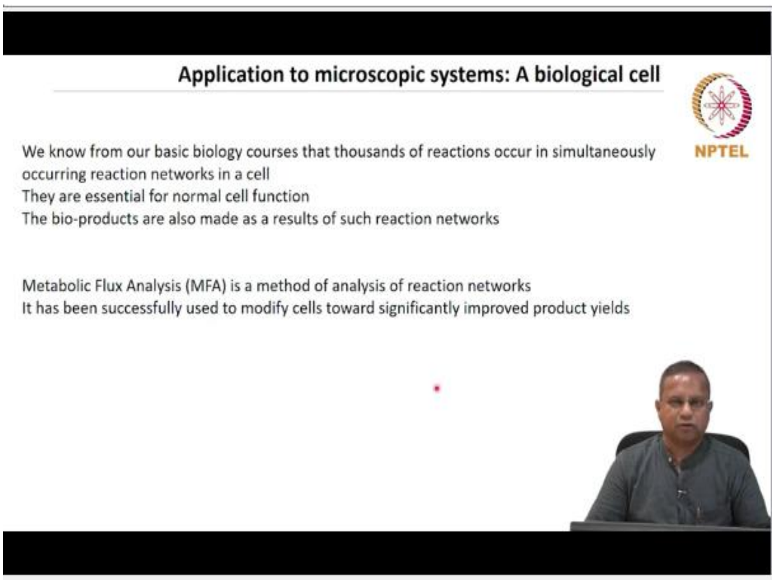

So, this is application to a microscopic system or a biological cell, where we looked at the reaction network in the cell and looked at the essence of metabolic flux analysis.

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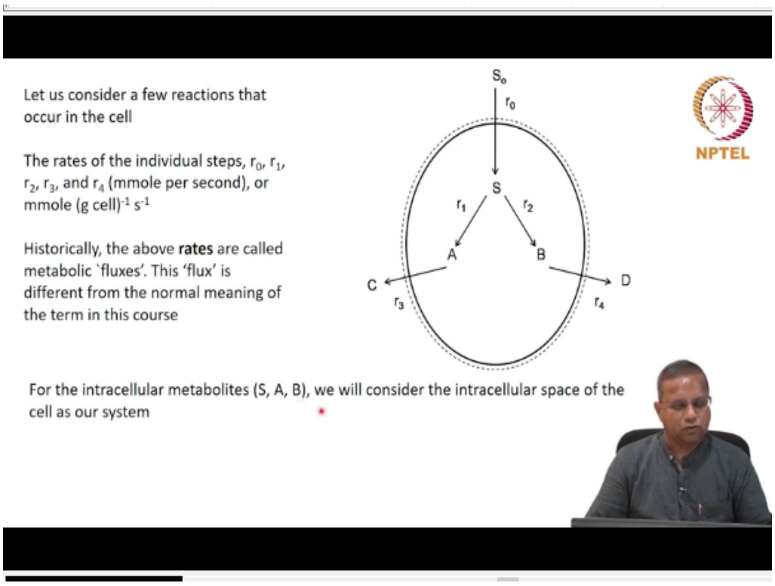

We considered a framework. We wrote the balances for each of these components in the framework. Okay, in the reaction framework. The trick that we used was that for the intracellular metabolites, we would use the inside of the cell as system for extra cell metabolites were used the outside of the cell as a system, the thing that we focus on.

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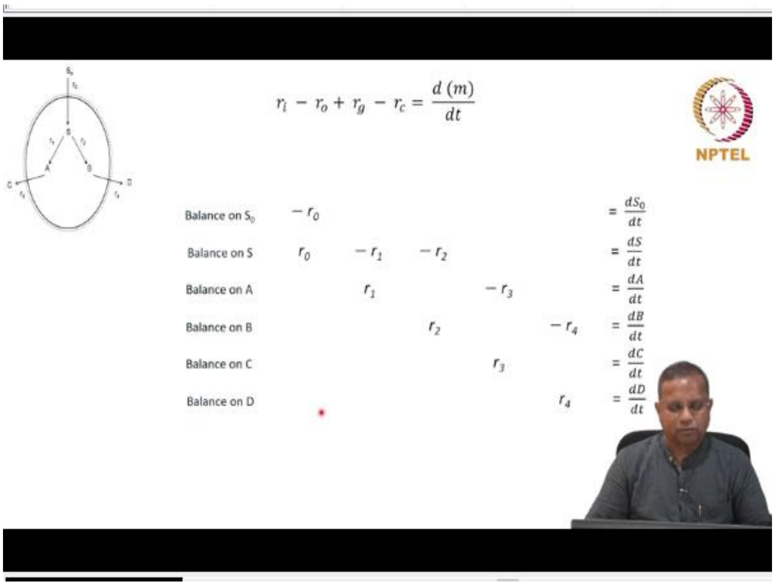

Then when we wrote the balances.

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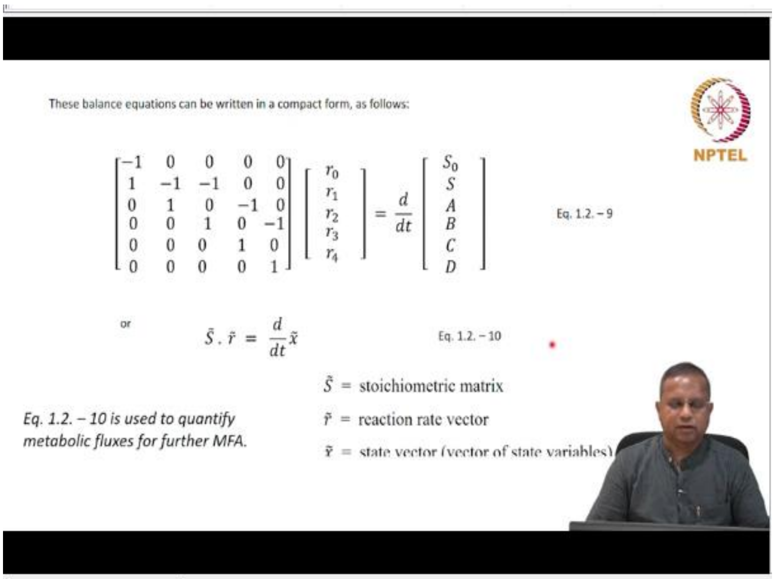

We could write it of the form that can be transferred to a compact matrix form, the stochiometric matrix, the rate vector and the vector of state variables the derivative of that is what the balance comes down to and this is very useful in different situations. You need of course, much more specifics to be able to make appropriate use of this formulation, okay. So, S.r = $\frac{dx}{dt}$, S matrix, r matrix or r vector and the derivative of this state variable vector.

So, stochiometric matrix, reaction rate vector and these state vector, vector of state variables. So, this is what we had seen. And then we started looking at fluxes, we defined what a flux was.

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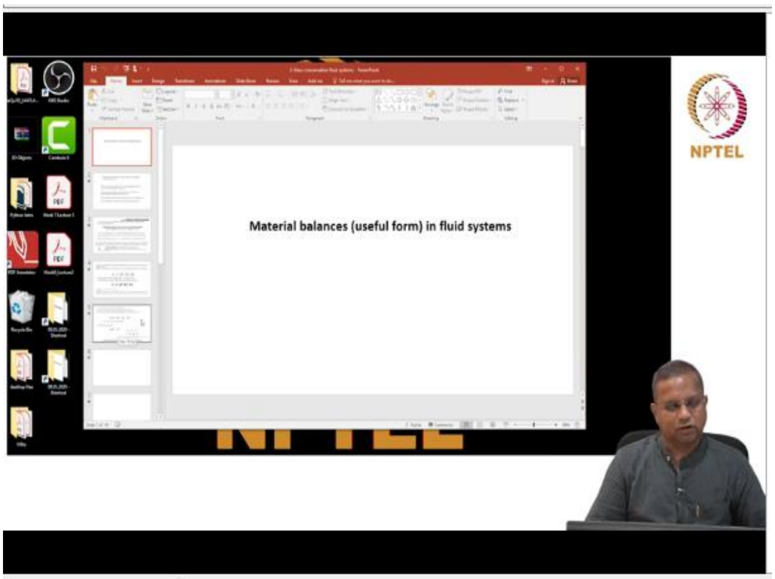

Before that we looked at mass conservation. So, I need to mention this.

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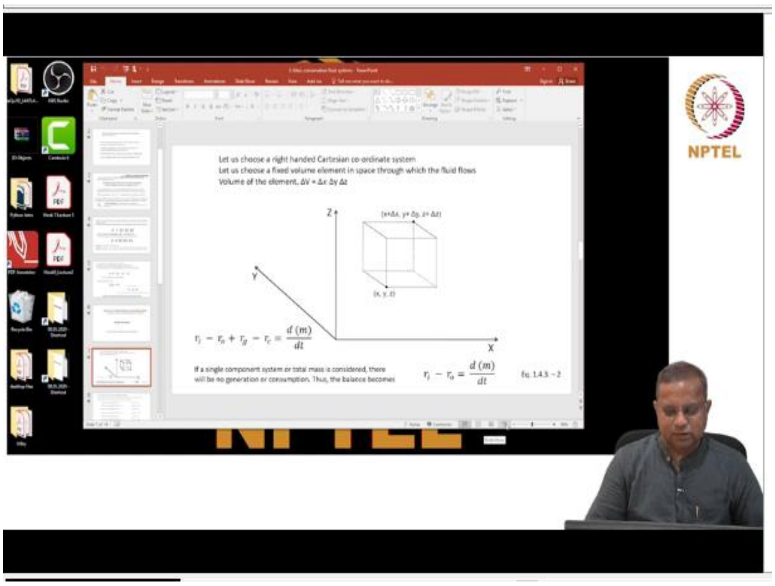

We considered a fluid flow situation.

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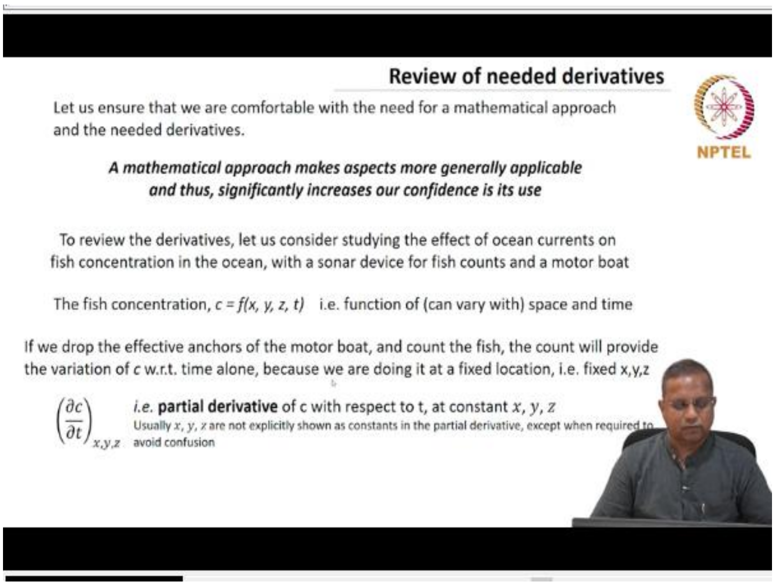

And then we said that we needed, we looked at derivatives that we needed and the review mode, partially derivative.

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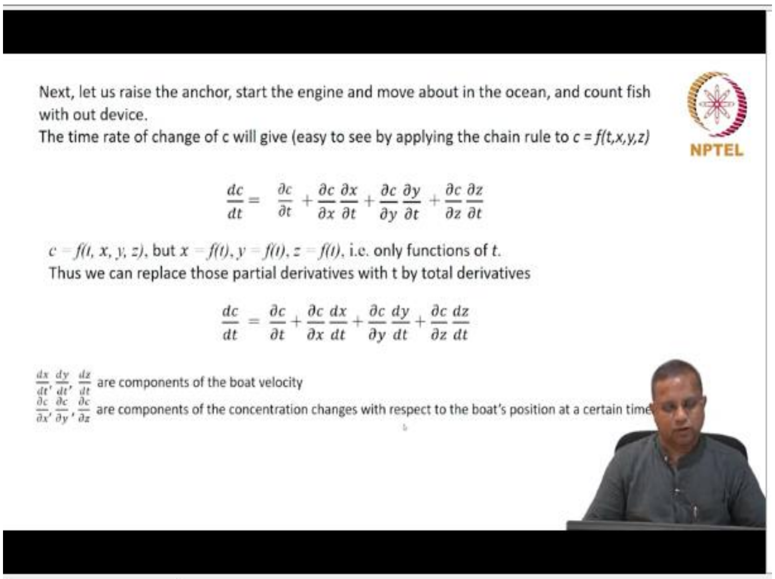

A total derivative and then we also looked at the substantial derivative which you may be familiar with or you may have picked up as a part of this course, okay.

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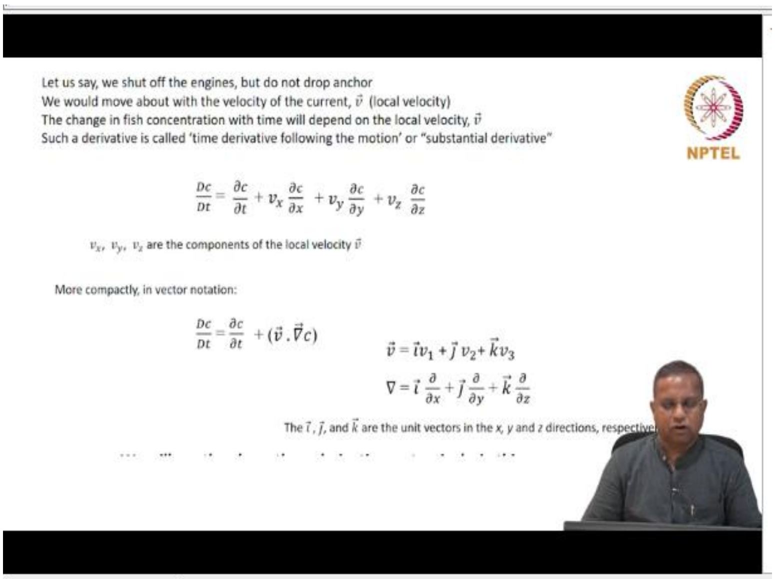

So, these are the 3 derivatives that would be used in this course, very useful derivatives and the compact notation that we can use, this is the equation of continuity for a single component system or the total mass taken in terms of substantial derivative here. That is what we had come to.

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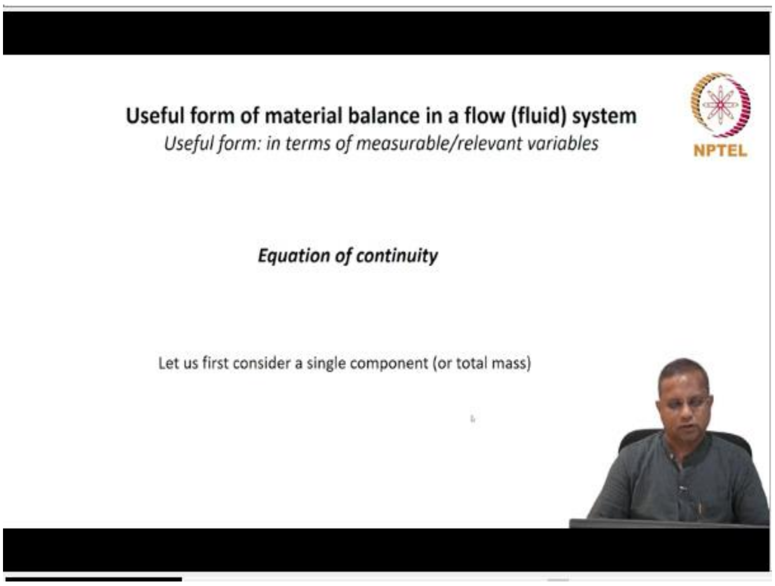

Before we got into the flux, you still follow the middle. Yeah, I had already given you a flavour of how things would be, we derive equations with a reasonably gentle have those tables, just refer to the tables, choose the appropriate equation, cancel out the relevant terms and go forward okay.

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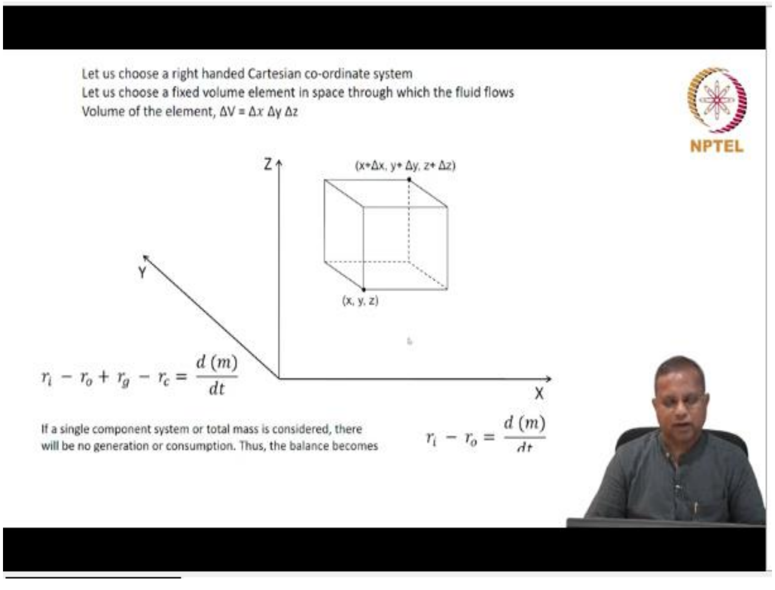

So, I have shown you the equation of continuity, derive the equation of continuity, take in the rectangular Cartesian coordinate system.

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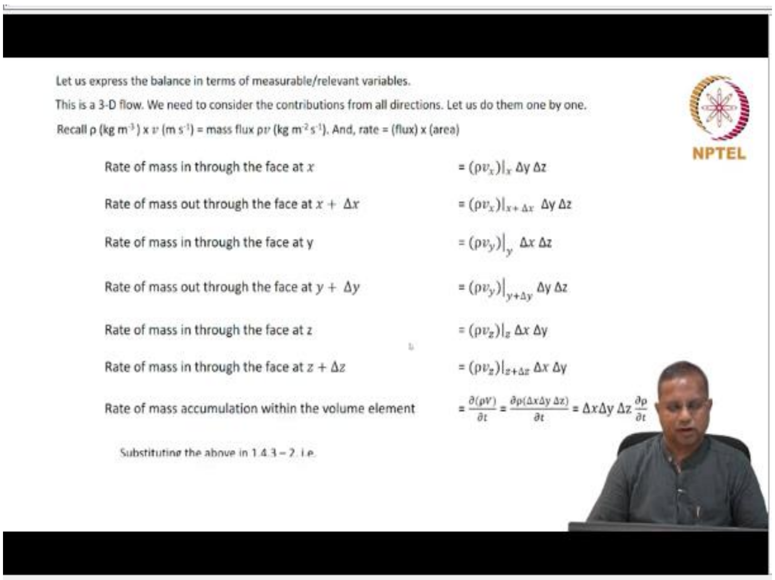

And extended that Cartesian.

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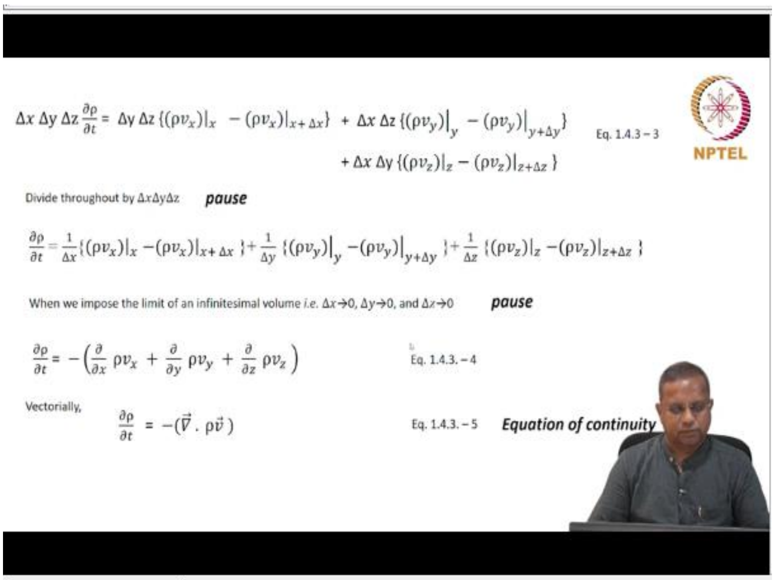

The equation of continuity to other coordinate systems.

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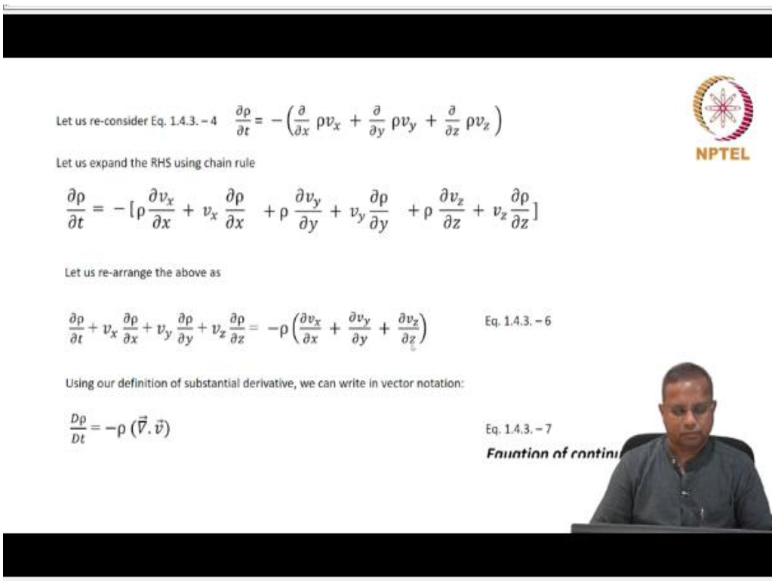

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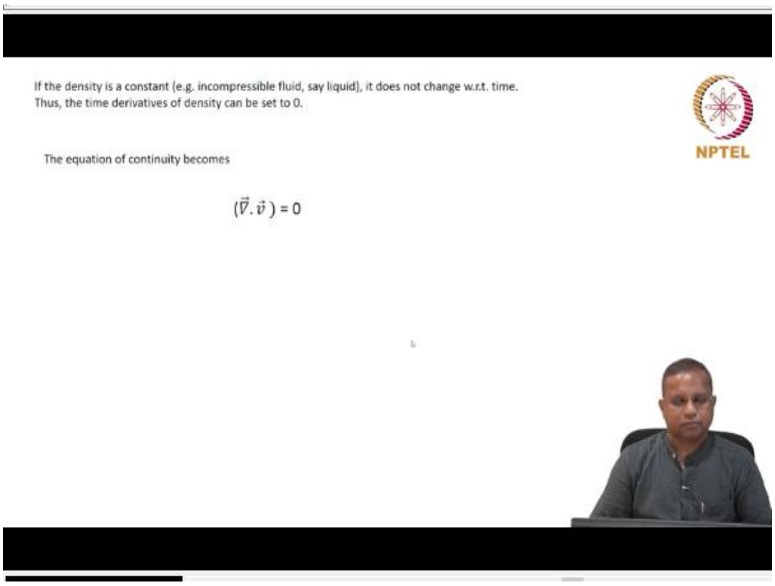

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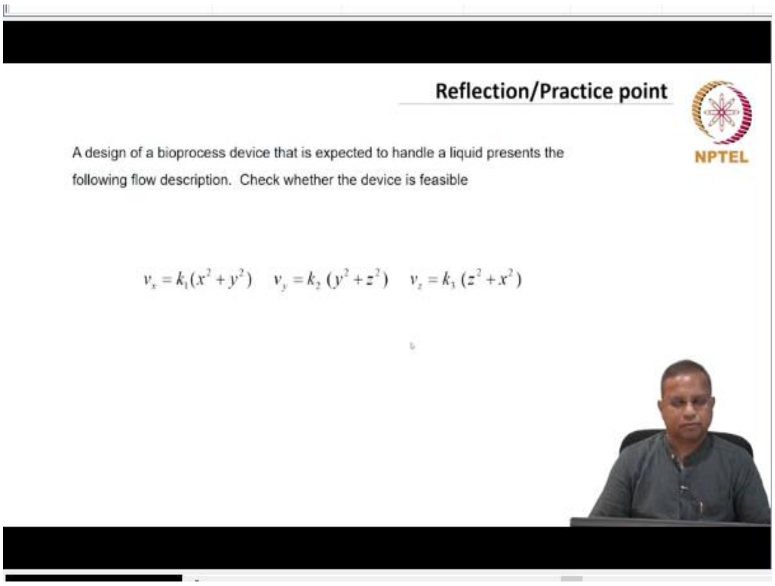

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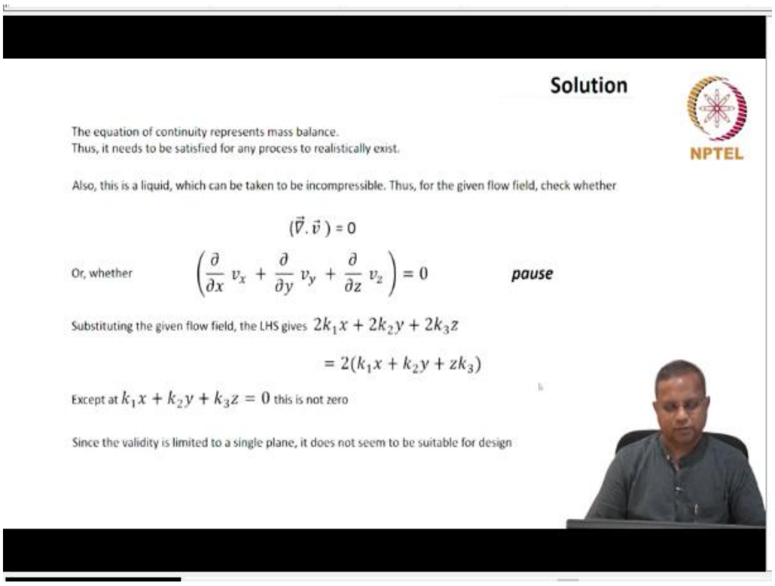

Okay.

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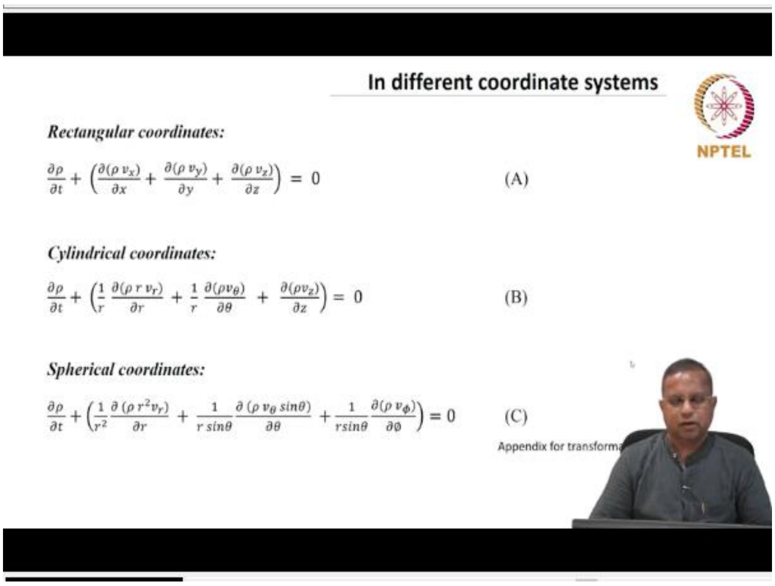

So, yeah, different coordinate systems. You have the rectangular coordinates here, which we derive. Then using the transformations in the appendix, it could go from the rectangle to the cylindrical coordinates from rectangle to the spherical coordinates. So, I would ask you to make a copy of this and keep it as a part of your notes to be used when there is a need okay. Then we started our mass flux.

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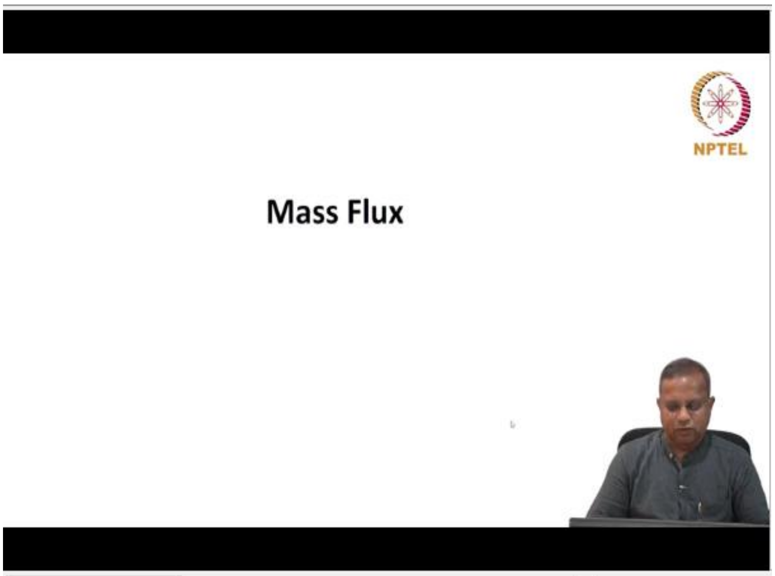

So, flux of any quantity.

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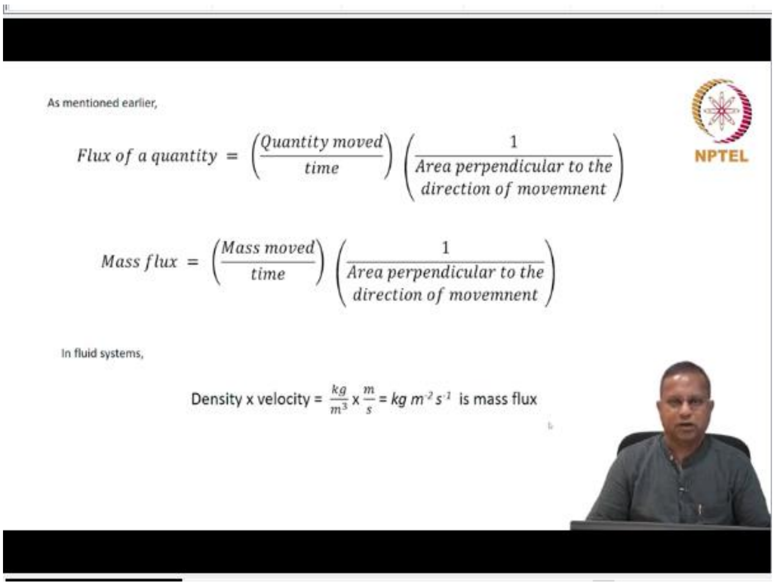

We have already seen was quantity mode per time, that was it is moving in this direction, per unit area that is perpendicular to the direction of motion. So, this was flux in this course, there were a few exceptions where the term flux was used differently, metabolic flux analysis was one such situation and the electric flux and magnetic flux from historical use of the term was a little different.

Apart from that, for this course, the flux meant this, quantity moved per time per unit area perpendicular to the direction of movement. Then, we said that the density times velocity is flux. We saw the various applications of this formulation, the basic formulation.

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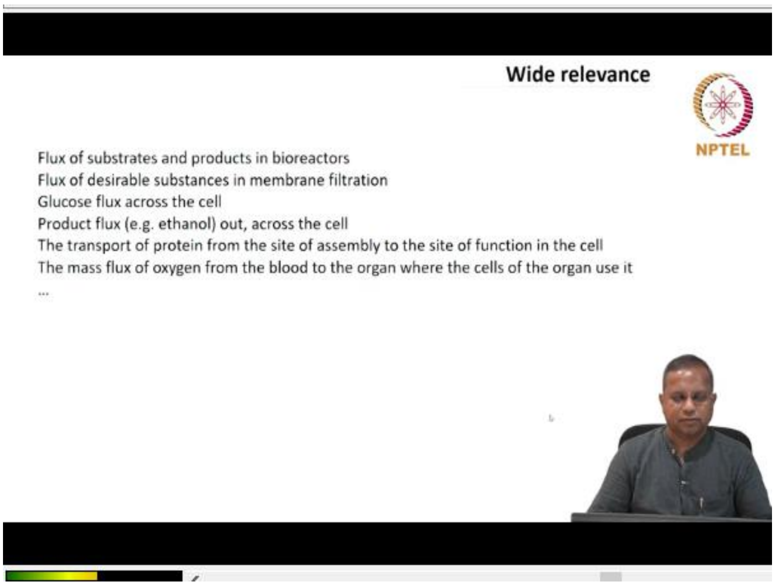

The definitions of average.

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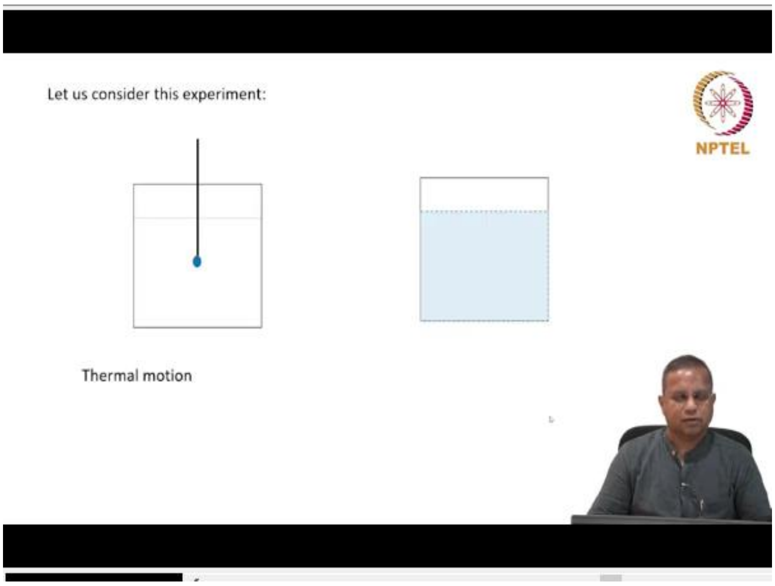

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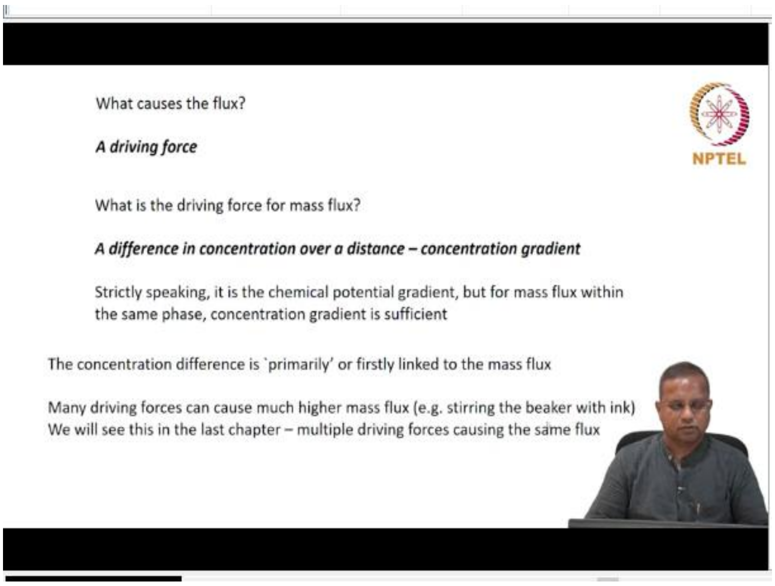

This is diffusion of course.

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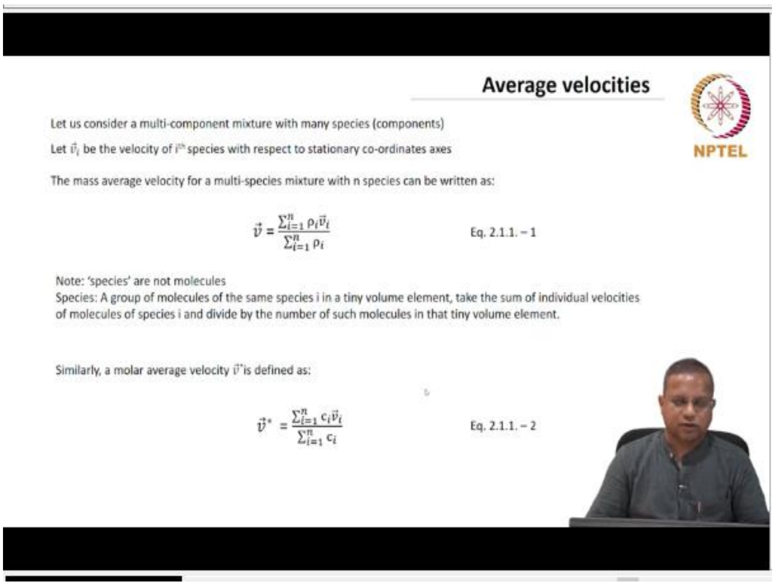

$$\vec{v} = \frac{\sum_{i=1}^{n} \rho_i \vec{v}_i}{\sum_{i=1}^{n} \rho_i} \qquad (2.1.1\text{-}1)$$

where ρ_i is the density of the i^{th} species.

.

$$\vec{v}^* = \frac{\sum_{i=1}^{n} c_i \vec{v}_i}{\sum_{i=1}^{n} c_i} \qquad (2.1.1\text{-}2)$$

where c_i is the concentration of species, i.

In a flowing system, the velocity of a species with respect to all species $\vec{v}$ or $\vec{v}^*$ is of more interest than the velocity with respect to stationary coordinates.

Thus, the useful quantities in such a system would be

$$\vec{v}_i - \vec{v} = \text{Diffusive velocity of } i \text{ with respect to } \vec{v} \qquad (2.1.1\text{-}3)$$

and

$$\vec{v}_i - \vec{v}^* = \text{Diffusion velocity of } i \text{ with respect to } \vec{v}^* \qquad (2.1.1\text{-}4)$$

This equation do not worry about the equation numbers. So, these 2 basic definitions we gave and expressed various quantities in terms of the mass average velocity, molar average velocity and so on and so forth.

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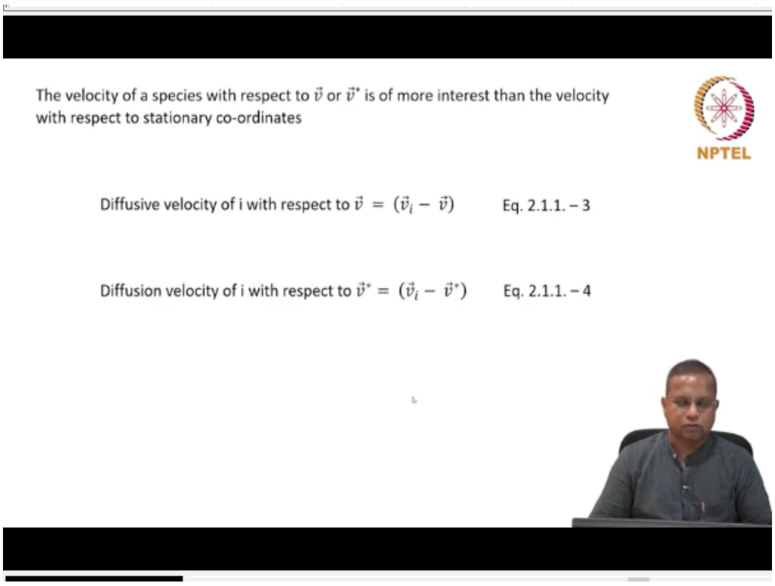

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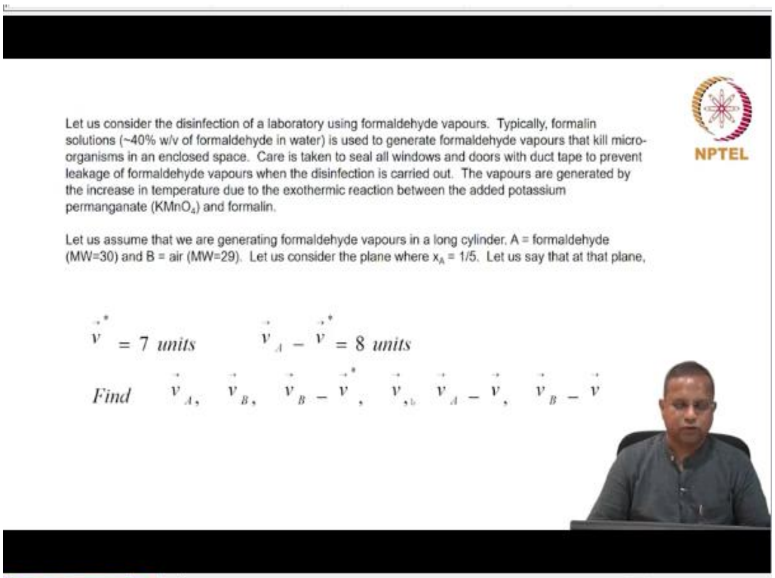

We went through a few exercises of those.

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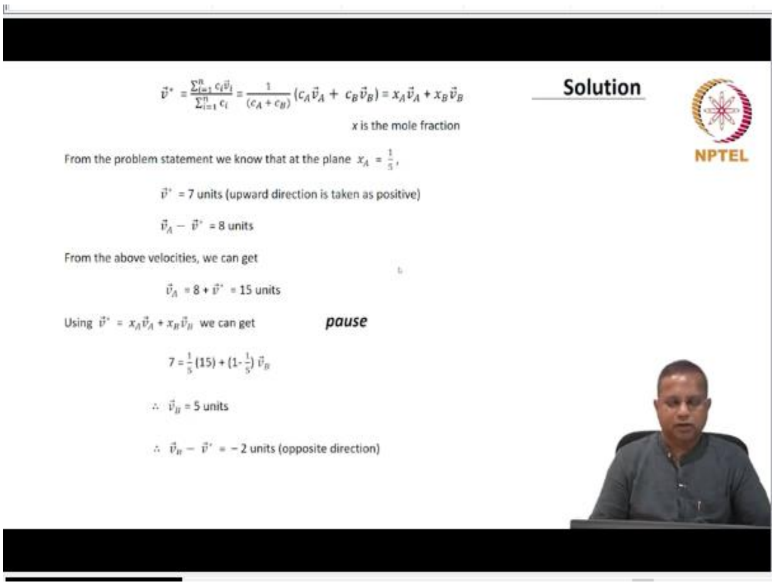

Okay we applied it to a situation that normally happens in the lab and that has been our approach you know integrate the problem solving, looking at things from the point of view of problems and so on and so forth. As a part of the basic learning itself.

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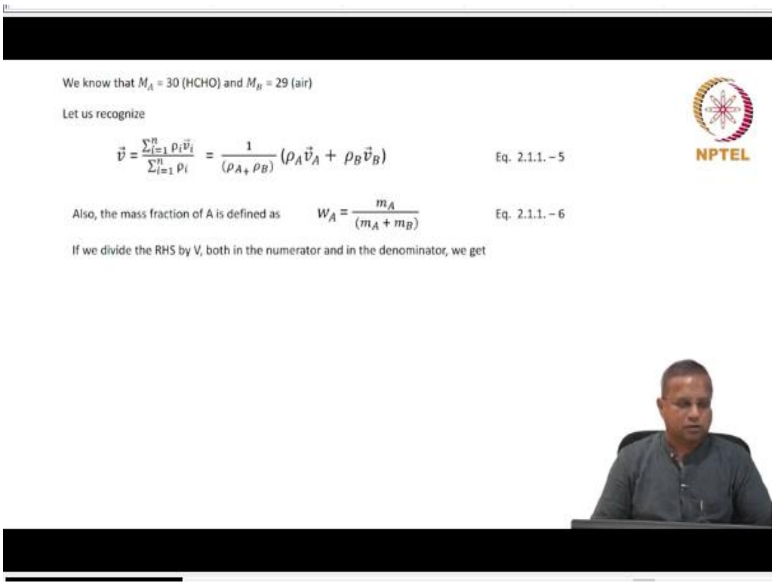

Then, we said there are 2 basic approaches to solve the relevant problems, okay, typically, we look for concentration profiles, when we solve mass balance, when we apply mass balance to these situations, because concentration profiles give us a lot of useful information. So, to do that, there are 2 major approaches.

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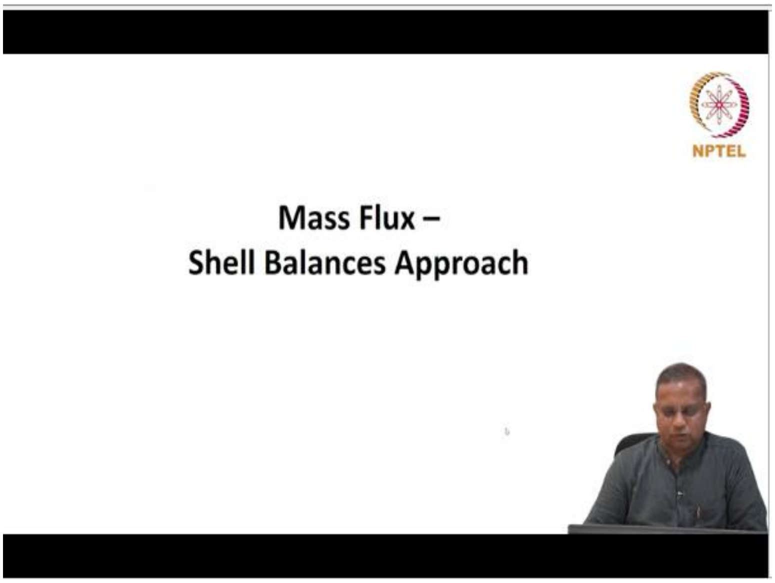

One is the shell balances approach.

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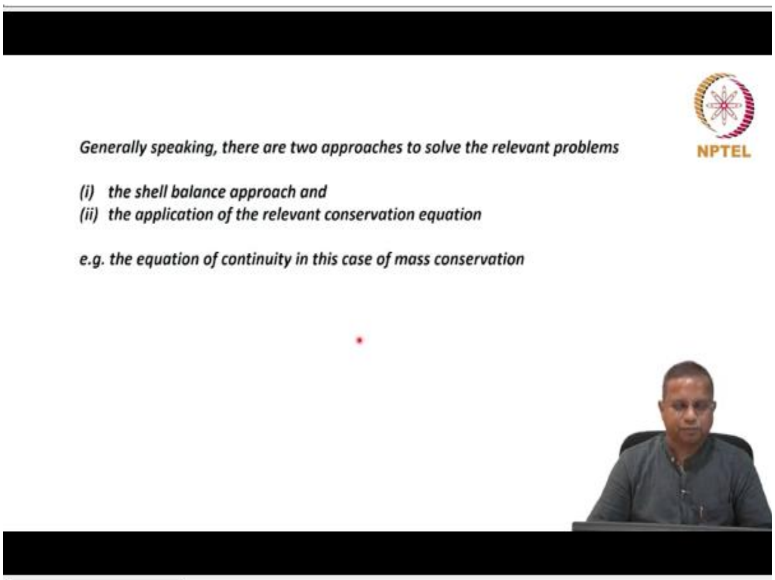

And the other one is the application of the relevant conservation equation approach. We said that the shell balance approach gives us good physical field for the situation. However, in geometries that are different from the rectangular Cartesian coordinate systems, they could get cumbersome and therefore, we looked at a relevant conservation equation that was reasonably gentle, which could be derived which could be set aside in a table.

And that can be referred to directly, you take that equation cancel out the terms it becomes a risk to be kind of a thing that you could do, much easier to work with. So, that is the relevant conservation equation approach. In the case of cell balances, we did balances over a representative shell in the fluid.

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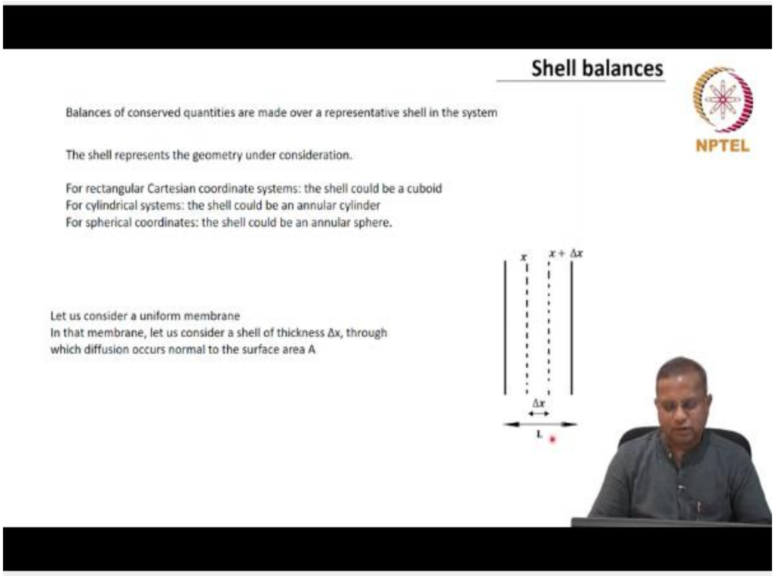

Balances over of conserved quantities are made over a representative shell in the system. The shell depends on the geometry under concentration and so on and so forth. So, here we had looked at a uniform membrane, diffusion through a uniform membrane, and the shell was a part of the membrane therefore, it was a thin cuboid in a membrane itself with a differential cuboid in a membrane of thickness Δx.

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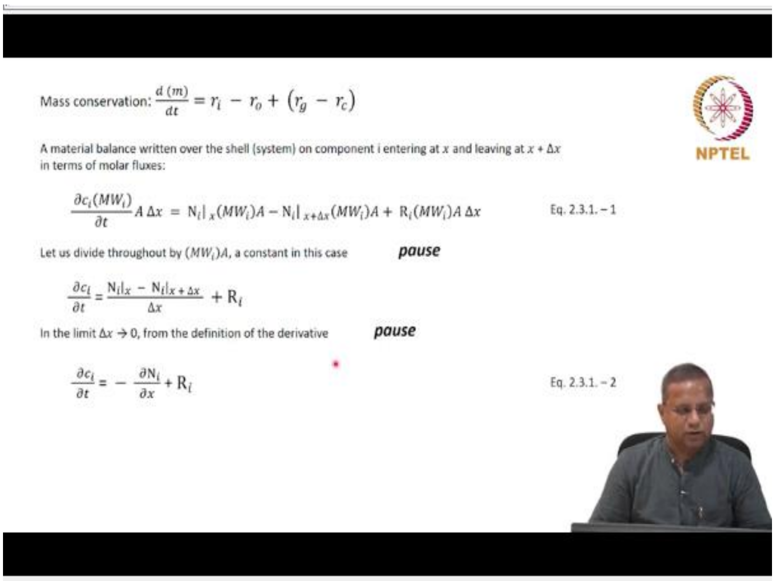

Over which we wrote our mass conservation balance. Then we wrote the balance in terms of the quantities that we have a handle on in terms of fluxes, molecular mass and so on. Even fluxes become a little difficult. Therefore, we wanted fluxes in terms of concentration and so on.

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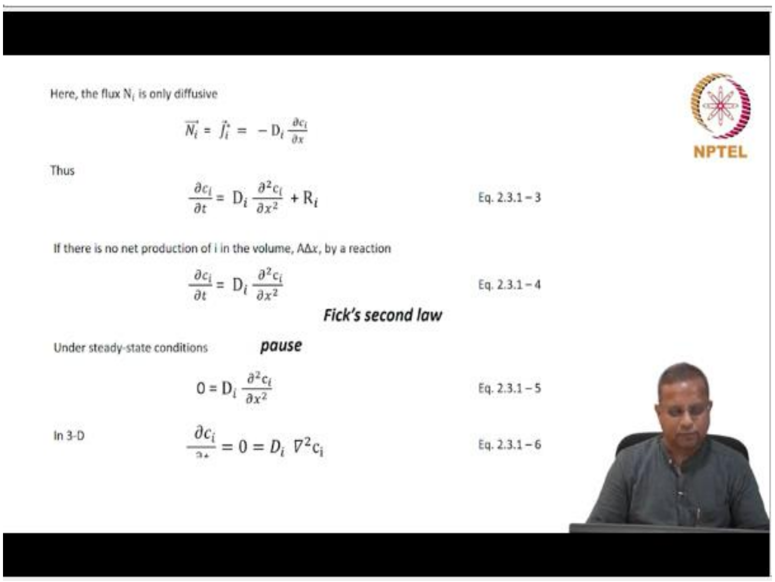

So, we derived the mass balance equation in detail. And for this situation, we could look at the concentration profile as well as the Fick's second law,

Under steady state conditions (no time dependence i.e. concentration does not vary with time), the LHS of Eq. 2.3.1-4 becomes zero. Thus

$$0 = D_i \frac{\partial^2 c_i}{\partial x^2} \qquad (2.3.1\text{-}5)$$

Equation 2.3.1-5 is the one-dimensional diffusion equation under steady state conditions with no reaction.

In three dimensions, under the same conditions, Fick's second law can be written as

$$\frac{\partial c_i}{\partial t} = 0 = D_i \nabla^2 c_i \qquad (2.3.1\text{-}6)$$

This is the governing equation which is called Fick's second down. Then, under steady state conditions, we saw the concentration profile of the species in the membrane in the system of interest.

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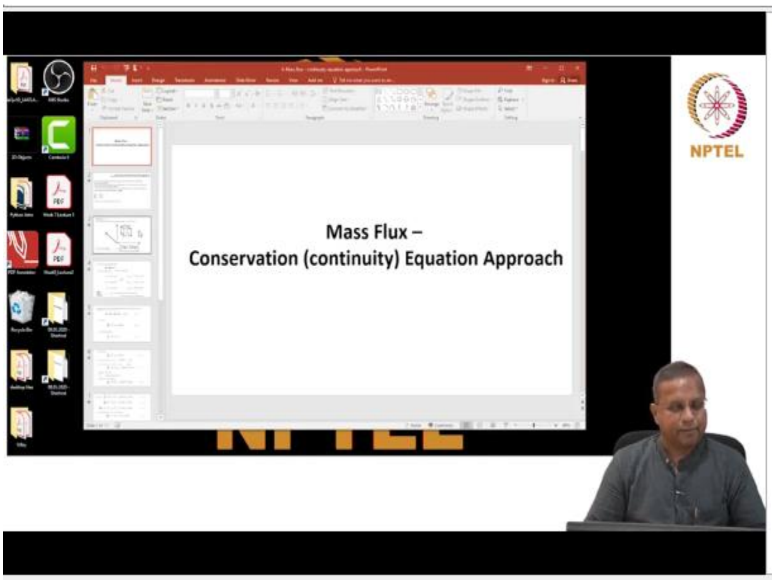

Then after deriving this equation, this is shell balances then we derive the equation let me show just the outlines of the derivation.

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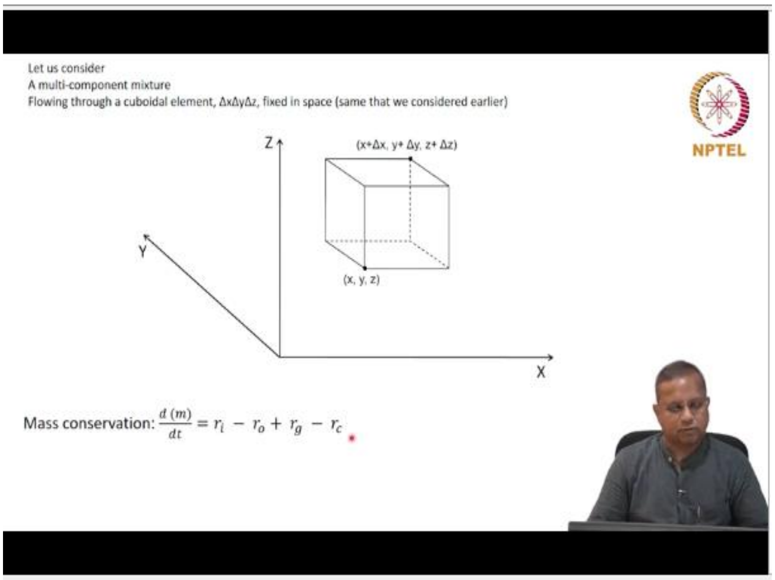

We are considered the rectangular Cartesian coordinate system. And same system as earlier in this case, we are considered a species. When we consider the species there could be an input, there could be an output, there could be generation of the species due to reaction, or there could be a consumption of the species due to reaction.

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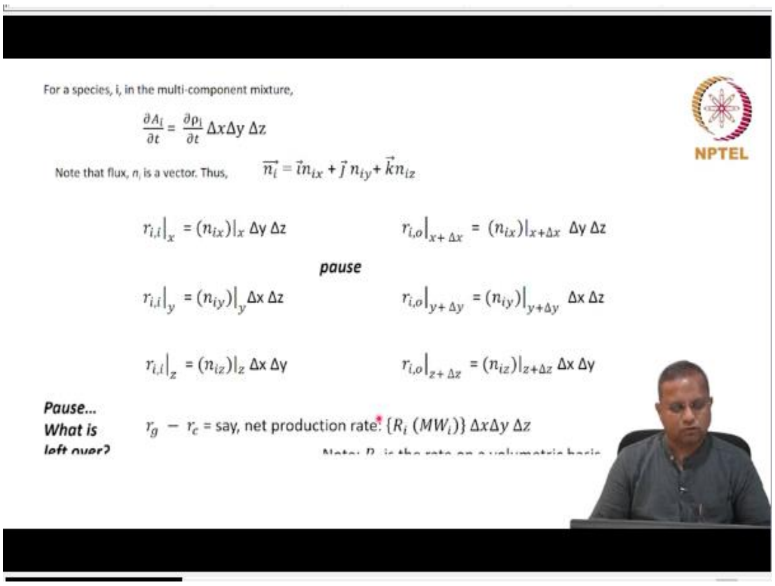

And then we derived a general enough relationship by considering all those.

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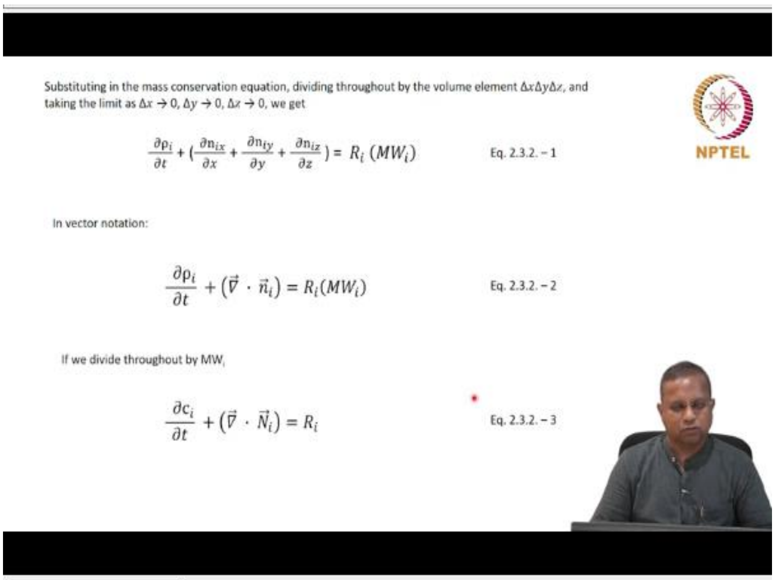

Okay. In detail, whenever there is a need, you can go through the details to find out.

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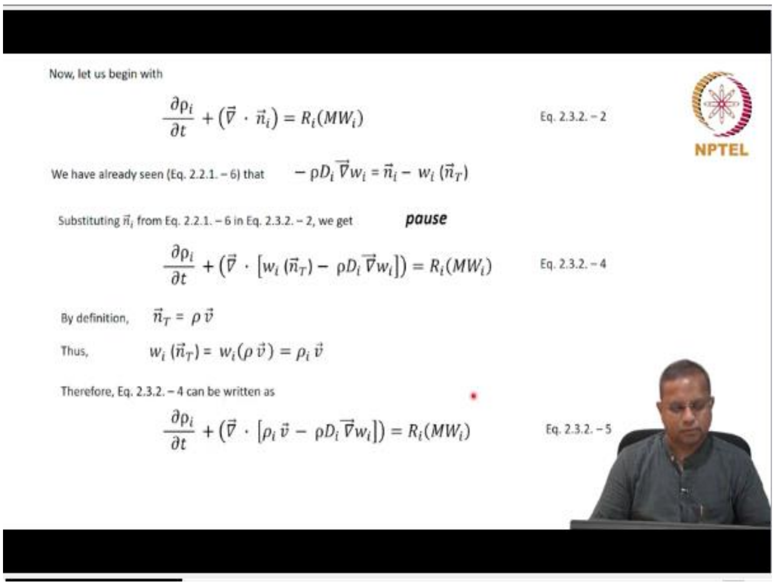

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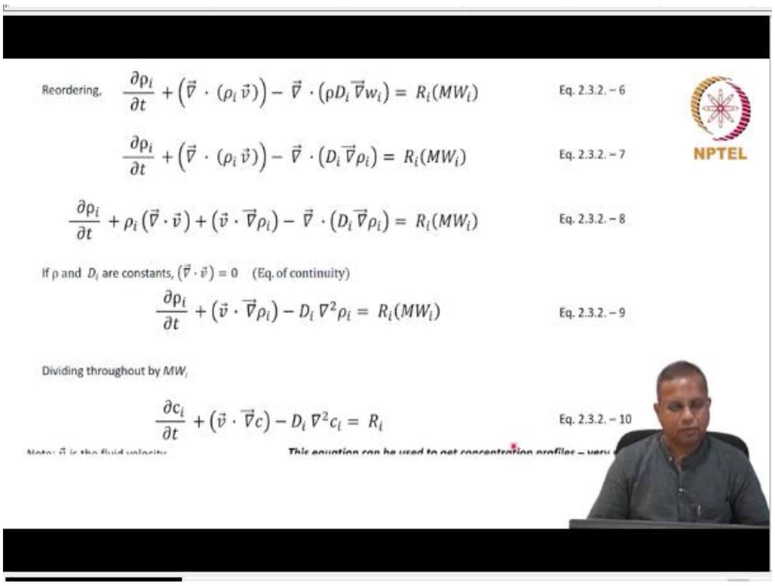

So, this form we said would be useful to us therefore, we express these in individual dimensions. And those became a part of a table in the 3 coordinate systems.

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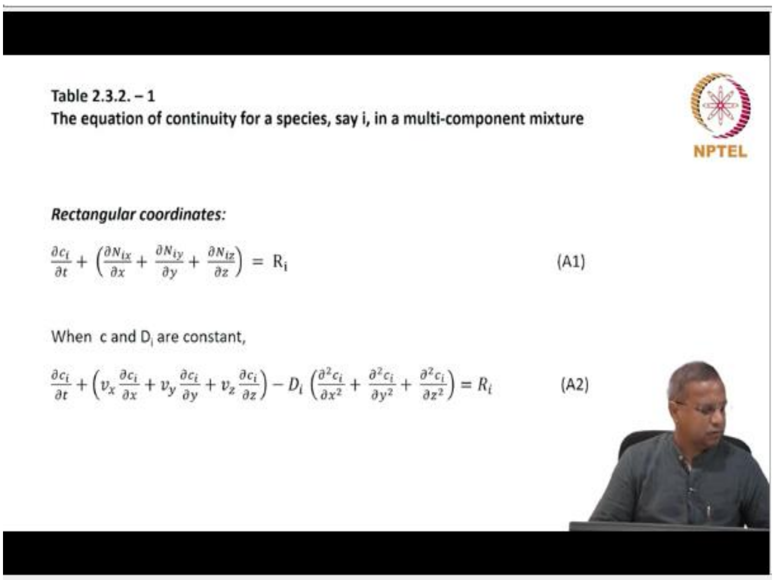

So, these were the tables that I showed you and asked you to make a copy of and keep at readily accessible place whenever you are looking at this material. And then I showed you the application of these equations to various situations. The first one was the problem that we solved by shell balances.

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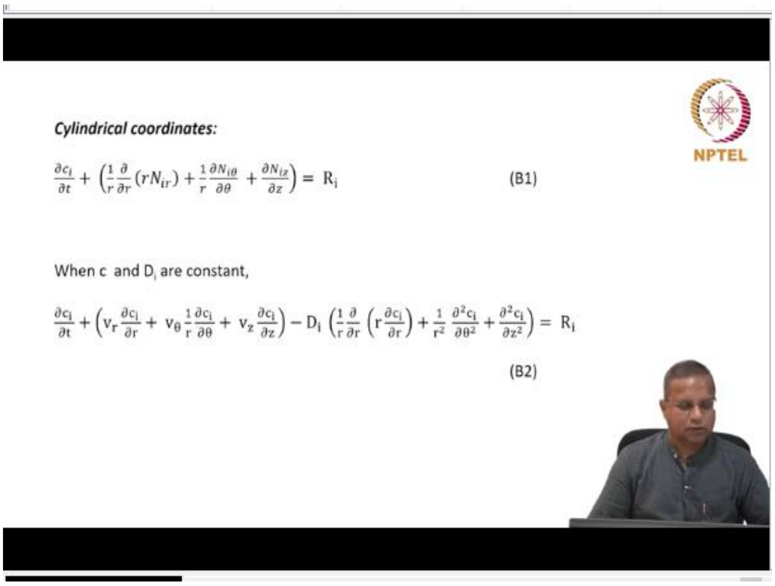

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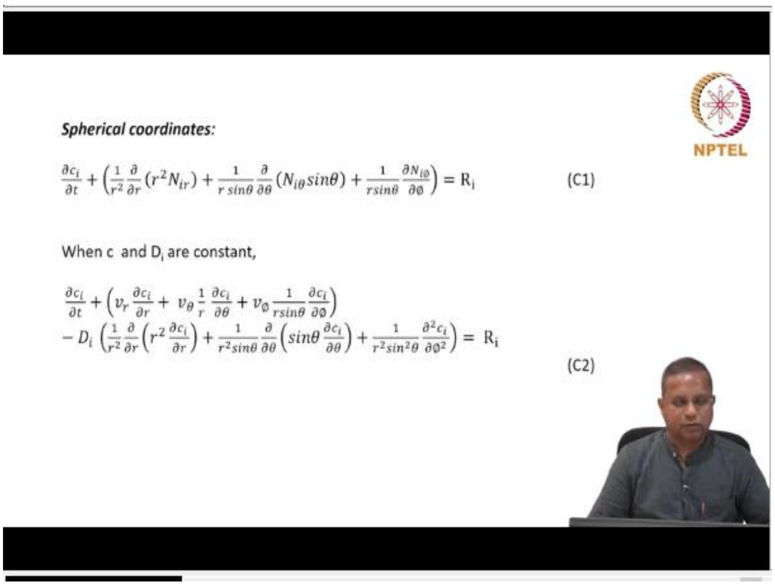

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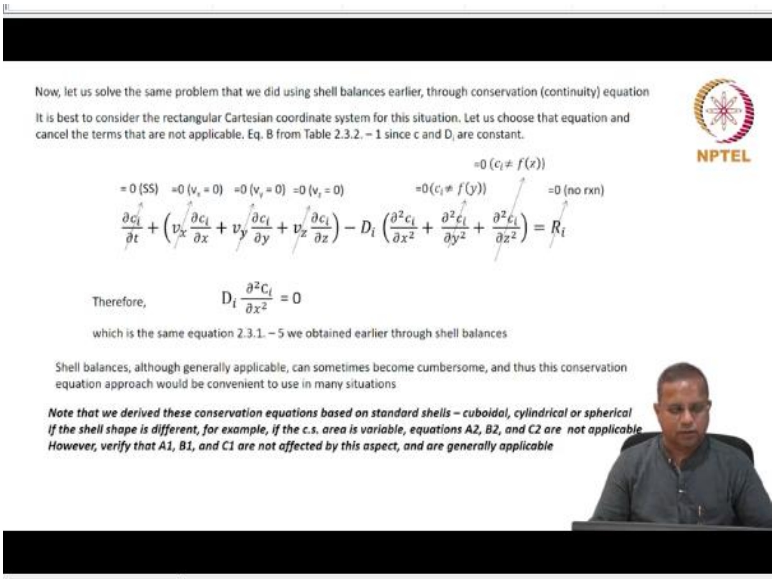

I showed you how very simply speaking, you just take the equation, you cancel the irrelevant terms. And at one swell step, you get the equation that we got through a lengthy derivation through shell balances, okay, this is the advantage of using one such thing therefore it is already gone into deriving a general enough equation which can be applied. Because this equation does not hold when there is a change in your cross section, over your system of interest and so on and so forth. You need to keep that in mind.

Then, we had applied to various situations. The first one was of course, the rectangle Cartesian coordinate system case, then we had used it to look at steady state diffusion of certain species across walls across membranes, then across tubular walls, we looked at the trachea sorry the bronchiole and a drug distributing from the inside of the bronchiole to the outside.

How do you look at that, and then we looked at diffusion through spherical porous pellets. And then these 3 were without reaction, then we brought in a reaction and looked at an enzymatic reaction where the enzyme is immobilized inside a porous pellet. So, that is the application of the equations to the 3 different geometries. And then we looked at an unsteady case where once you bring in an unsteady term, the time derivative, it complicated the mathematical effort significantly, okay.

And as all those things we saw, the unsteady state case was, we had a protein solution that is solving onto a surface. And we were interested in the concentration profiles in that quiescent liquid about the surface, the variation of the concentration profiles with time. Okay, those are the things that we saw.

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And finally, let me have been at this for a while, I think we should stop to avoid fatigue. I will just say this. It is important. Then we will stop for today and continue in the next class. Okay. So, we also looked at a very powerful approximation, a very powerful idea, called the pseudo steady state approximation.

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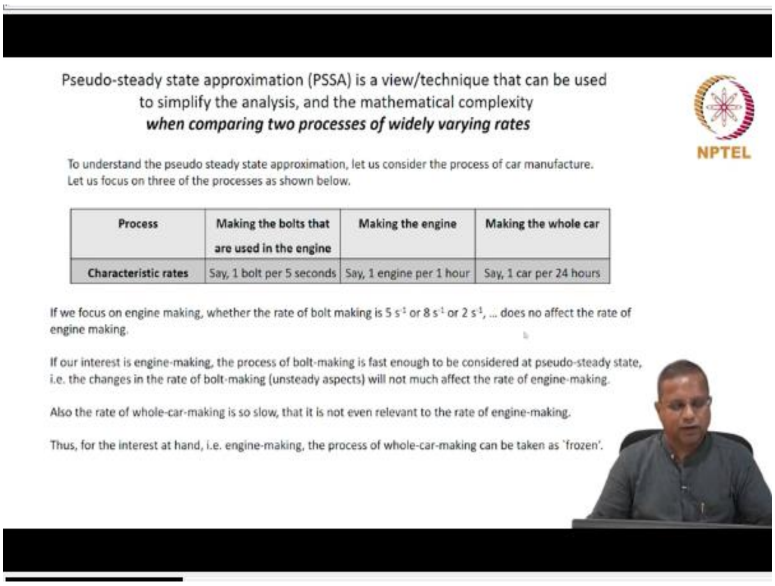

It is something like this when you have, when you are comparing to processes of widely varying rates, the much faster process can be taken to be at steady state, if the interest is this slower process.

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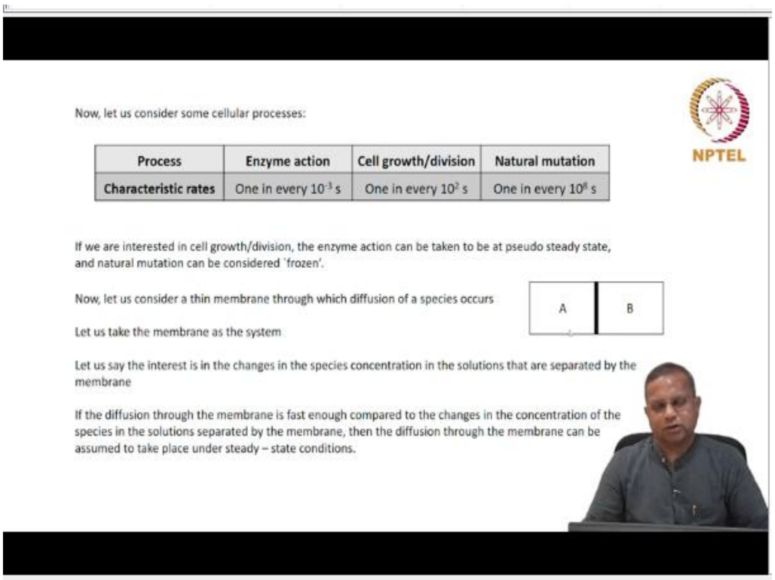

So, we had applied this to come up with the permeability of a coating layer, when the permeability through the coating layer is of interest, the experiment that is done as measuring permeability of a mechanically stable membrane, and then you put the coating layer onto the membrane and measure the combined permeability.

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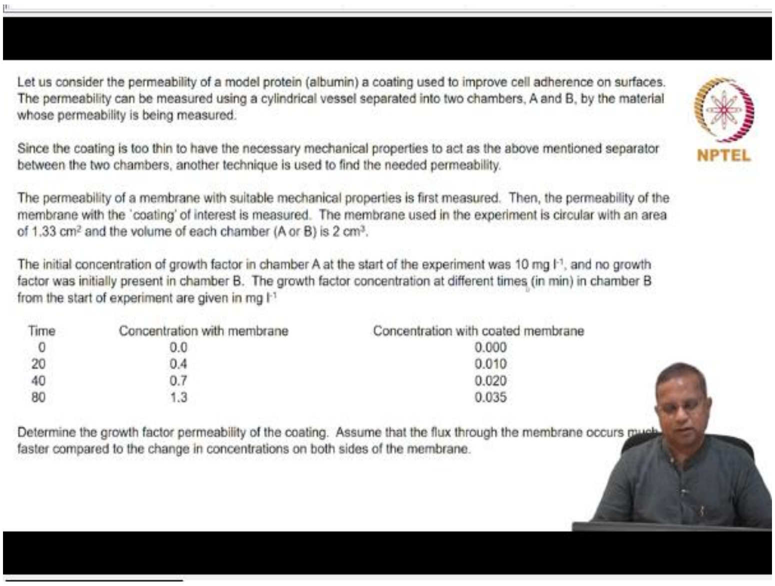

And from that data to extract out the relevant membrane permeability, we had to use the pseudo steady state principle and get the permeability.

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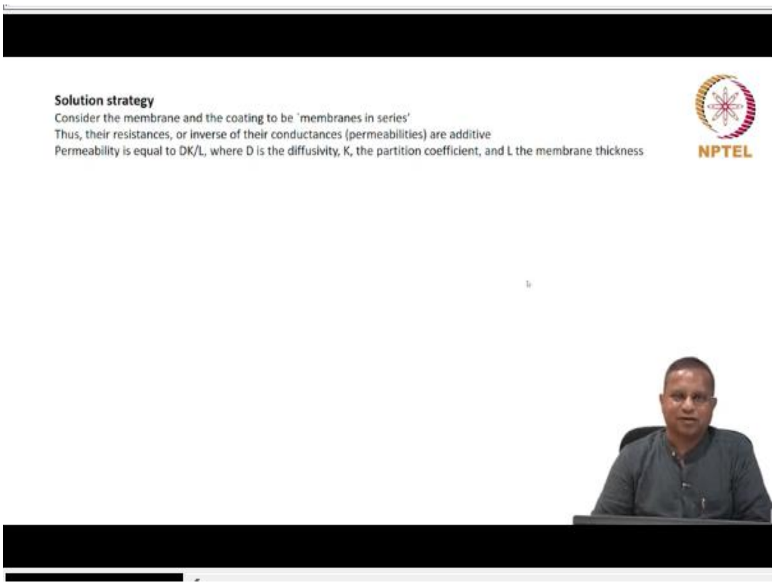

That is what we had seen. That was the example that was given. The pseudo steady state concept itself was a very powerful concept that can be use in any situation whenever you compare to processes of widely varying rates and the interest is in the slower process. Okay. I think that is what we did for mass flux, mass transport, mainly through diffusion okay, there is no mass flux through bulk movement.

Although the equations that were derived had the ability to handle that also. But for better understanding, we just forced the driving force to a concentration gradient. In all these cases, we took examples here only the concentration gradient was the driving force, and showed you the various applications of it. When we come back in the next class, we have been at this for a while now and we come back, we would look at momentum flux, review that and forward. See you in the next class. Bye