Transport Phenomena in Biological Systems
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Lecture-81
Course Review-Part 4

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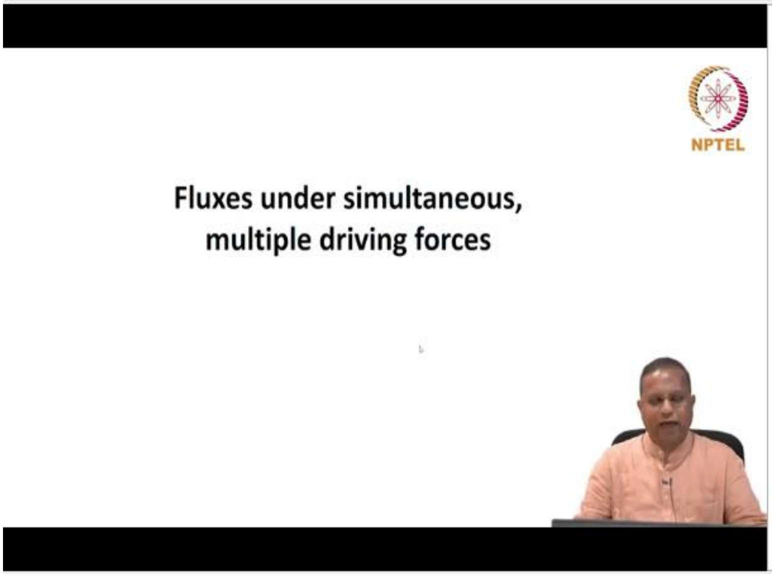

Fluxes under simultaneous, multiple driving forces

Welcome to the last review lecture, we are going to review the final chapter the fluxes under simultaneous multiple driving forces.

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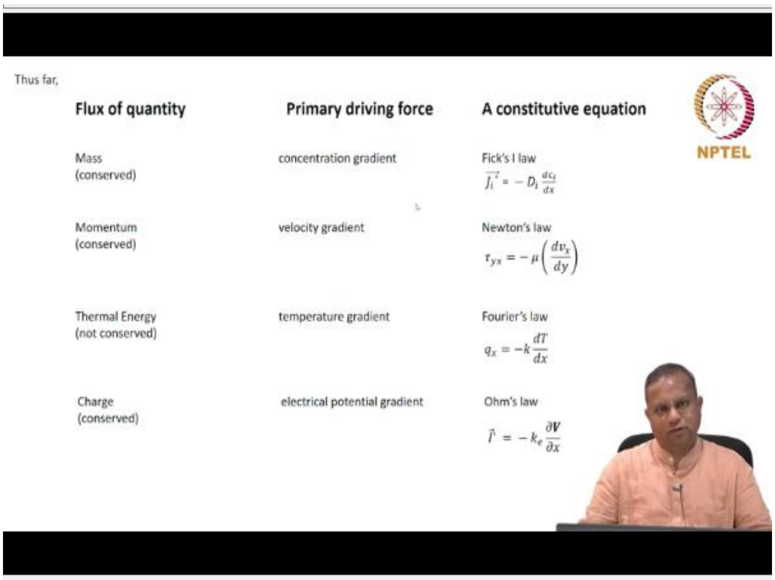

Thus far,

Flux of quantity	Primary driving force	A constitutive equation
Mass (conserved)	concentration gradient	Fick's I law $\vec{J_i^*} = -D_i \frac{dc_i}{dx}$
Momentum (conserved)	velocity gradient	Newton's law $\tau_{yx} = -\mu\left(\frac{dv_x}{dy}\right)$
Thermal Energy (not conserved)	temperature gradient	Fourier's law $q_x = -k\frac{dT}{dx}$
Charge (conserved)	electrical potential gradient	Ohm's law $\vec{I} = -k_e\frac{\partial V}{\partial x}$

When we began the review, I had shown you this right, this pretty much gives you the crux or the essence of the entire course. If you look at the flux of a quantity, primary driving force constitutive equation, let me just quickly run through this we have already discussed this. We looked at concentration gradient as the primary driving force for mass flux and a constitutive equation the Fick’s law.

The velocity gradient as the primary driving force for a moment flux, Newton's law as a constitutive equation, temperature gradient, the primary driving force with thermal energy, Fourier’s law as a conservative equation, electrical potential gradient as the primary driving force with charge flux with ohms law as a constraint equation okay. So, you can see the relationship between the various fluxes.

The forms of equations are all similar, which relate this in this and the forms of even the constitutive equations are examples of constitutive equations are also very similar, okay. At least the simplest conservative equations are all very similar in their form okay, only thing is that the details are different. So, this is so far in the course and in this chapter we are going to look at multiple driving forces causing a flux or multiple fluxes.

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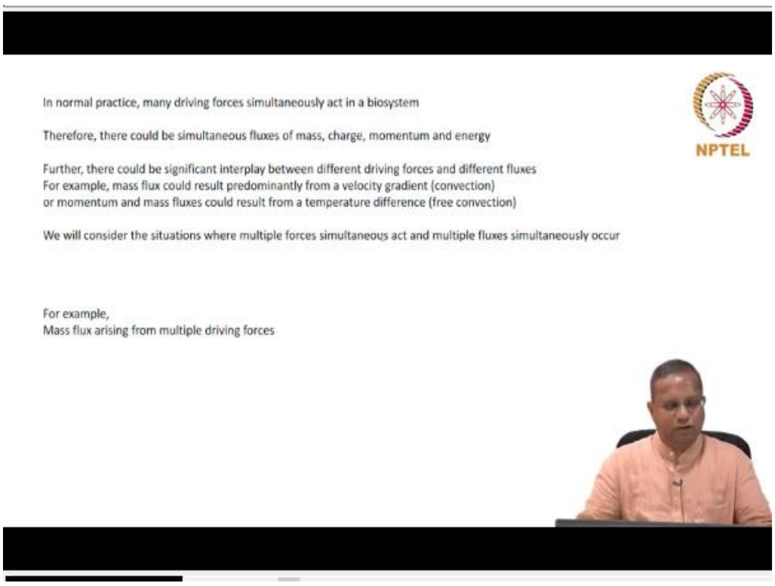

In normal practice, many driving forces simultaneously act in a biosystem

Therefore, there could be simultaneous fluxes of mass, charge, momentum and energy

Further, there could be significant interplay between different driving forces and different fluxes
For example, mass flux could result predominantly from a velocity gradient (convection)
or momentum and mass fluxes could result from a temperature difference (free convection)

We will consider the situations where multiple forces simultaneous act and multiple fluxes simultaneously occur

For example,
Mass flux arising from multiple driving forces

So, we said there are a few couple of ways by which you could approach this, one is since the fundamental equations were conservation equations, conservation of conserved quantities or the conservation of conserved physical quantities, that is what was represented in continuity equation of motion, equation of energy and the charge conservation equation. Therefore, they should certainly be applicable.

So, if there are multiple driving forces you write down all those equations and you could simultaneously solve them, in principle it should work okay. However, practically it could be mathematically complex, it could get very high and the solution could get very difficult.

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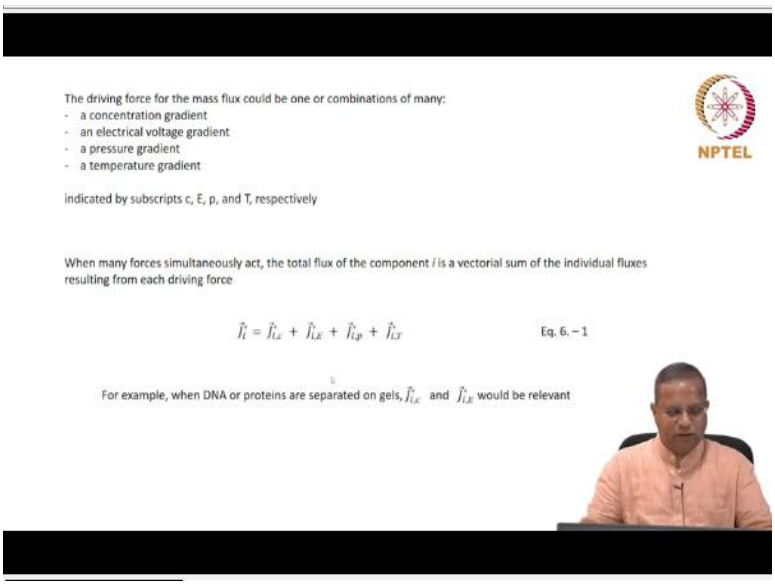

The driving force for the mass flux could be one or combinations of many:

- a concentration gradient
- an electrical voltage gradient
- a pressure gradient
- a temperature gradient

indicated by subscripts c, E, p, and T, respectively

When many forces simultaneously act, the total flux of the component *i* is a vectorial sum of the individual fluxes resulting from each driving force

$$\vec{J}_i = \vec{J}_{i,c} + \vec{J}_{i,E} + \vec{J}_{i,p} + \vec{J}_{i,T} \qquad \text{Eq. 6.-1}$$

For example, when DNA or proteins are separated on gels, $\vec{J}_{i,c}$ and $\vec{J}_{i,E}$ would be relevant

And therefore, we use a slightly different approach, which is the we just called the transfer coefficient approach right, you have a mass transfer coefficient heat transfer coefficient and so on and so forth, you could do that okay. So, we started by looking at an important aspect of mass flux under the influence of both potential gradient and a concentration gradient.

We spent a good amount of time on that, before that the mass flux could arise due to a concentration gradient, electrical potential gradient, pressure gradient flow as well as a temperature gradient natural convection okay, out of which we chose to look at 2 in this.

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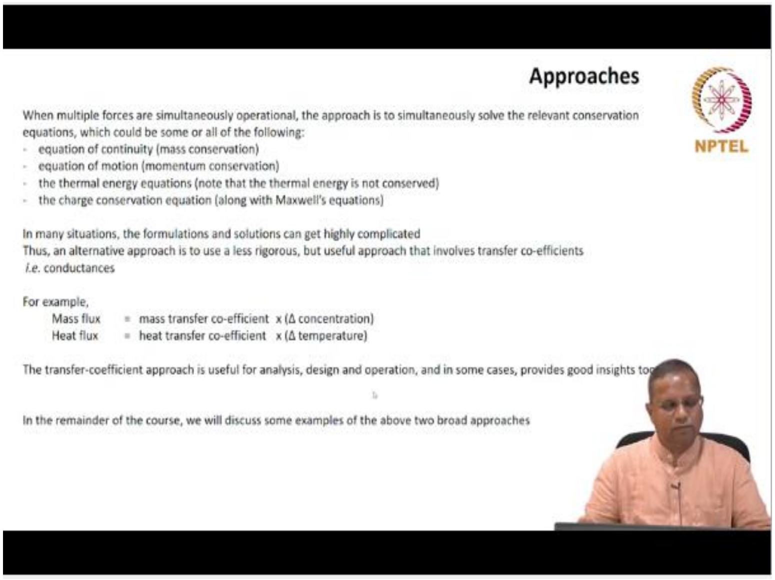

Approaches

When multiple forces are simultaneously operational, the approach is to simultaneously solve the relevant conservation equations, which could be some or all of the following:

- equation of continuity (mass conservation)
- equation of motion (momentum conservation)
- the thermal energy equations (note that the thermal energy is not conserved)
- the charge conservation equation (along with Maxwell's equations)

In many situations, the formulations and solutions can get highly complicated
Thus, an alternative approach is to use a less rigorous, but useful approach that involves transfer co-efficients
i.e. conductances

For example,
Mass flux = mass transfer co-efficient x (Δ concentration)
Heat flux = heat transfer co-efficient x (Δ temperature)

The transfer-coefficient approach is useful for analysis, design and operation, and in some cases, provides good insights to

In the remainder of the course, we will discuss some examples of the above two broad approaches

These were the approaches, mass flux, heat flux and so on and so forth. Mass transfer coefficient, heat transfer coefficient and so on.

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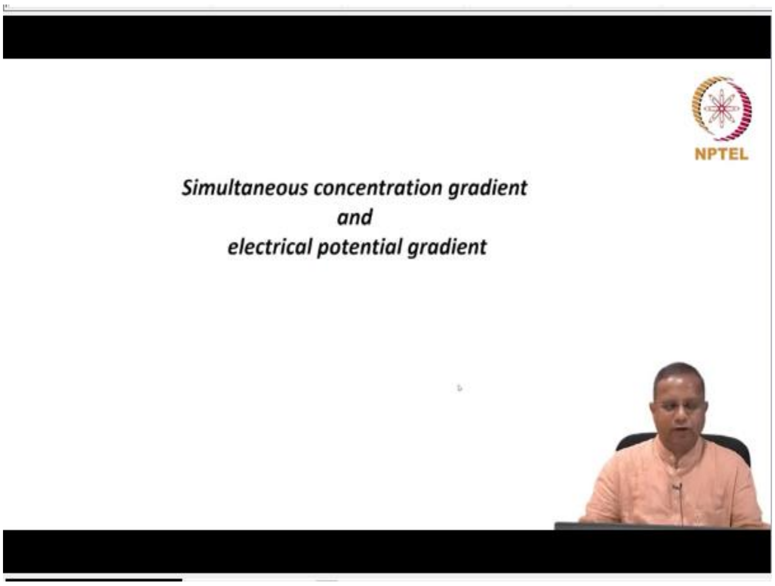

Simultaneous concentration gradient
and
electrical potential gradient

When we the concentration gradient and electrical potential gradient case was very interesting.

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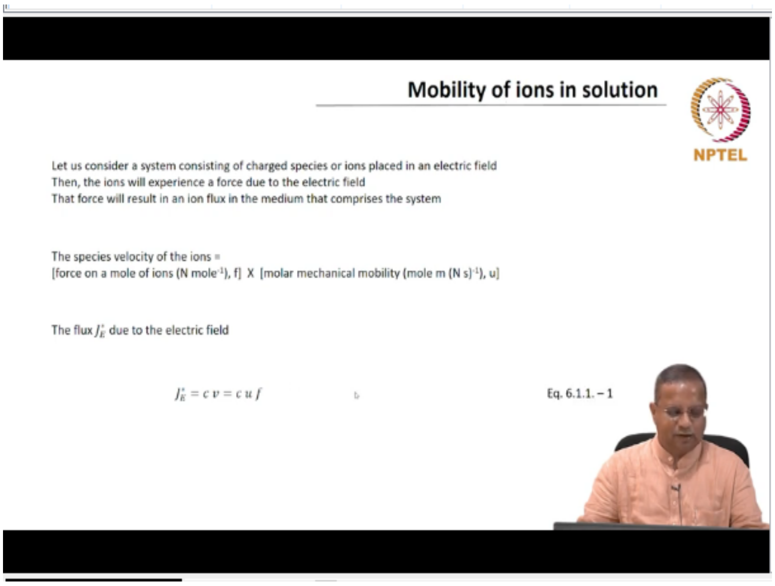

Mobility of ions in solution

Let us consider a system consisting of charged species or ions placed in an electric field
Then, the ions will experience a force due to the electric field
That force will result in an ion flux in the medium that comprises the system

The species velocity of the ions =
[force on a mole of ions (N mole^{-1}), f] X [molar mechanical mobility (mole m (N s)$^{-1}$), u]

The flux J_E^* due to the electric field

$$J_E^* = c\,v = c\,u\,f \qquad \text{Eq. 6.1.1.} - 1$$

We started looking at the mobility of ions in solution.

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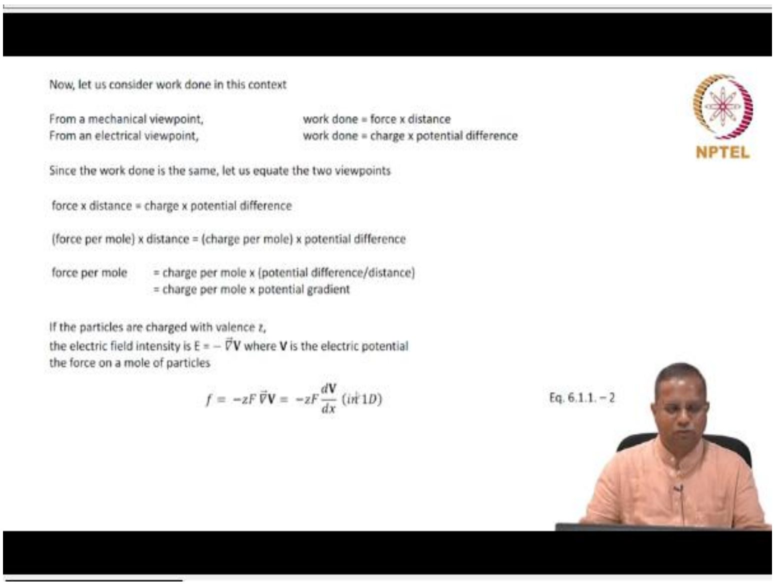

Now, let us consider work done in this context

From a mechanical viewpoint, work done = force x distance
From an electrical viewpoint, work done = charge x potential difference

Since the work done is the same, let us equate the two viewpoints

force x distance = charge x potential difference

(force per mole) x distance = (charge per mole) x potential difference

force per mole = charge per mole x (potential difference/distance)
= charge per mole x potential gradient

If the particles are charged with valence z,
the electric field intensity is $E = -\vec{\nabla}\mathbf{V}$ where $\mathbf{V}$ is the electric potential
the force on a mole of particles

$$f = -zF\,\vec{\nabla}\mathbf{V} = -zF\frac{d\mathbf{V}}{dx}\ (in\ 1D) \qquad \text{Eq. 6.1.1.} - 2$$

We started with very basic definitions.

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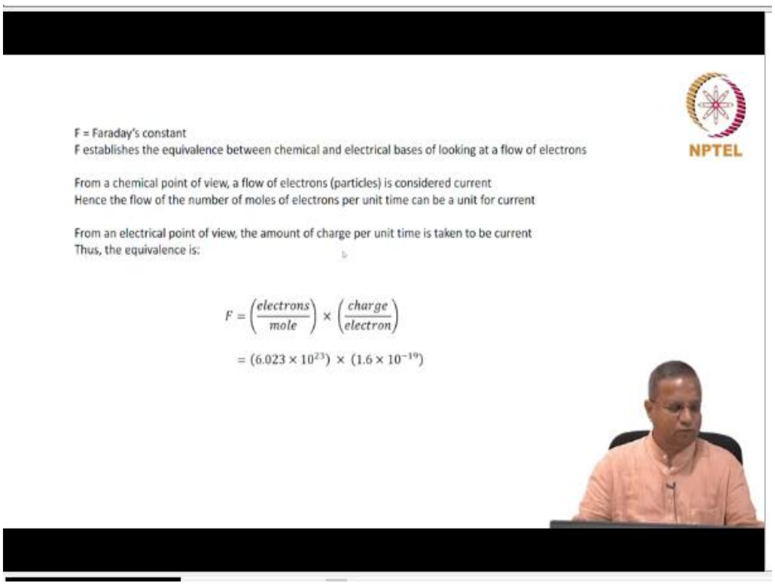

F = Faraday's constant
F establishes the equivalence between chemical and electrical bases of looking at a flow of electrons

From a chemical point of view, a flow of electrons (particles) is considered current
Hence the flow of the number of moles of electrons per unit time can be a unit for current

From an electrical point of view, the amount of charge per unit time is taken to be current
Thus, the equivalence is:

$$F = \left(\frac{electrons}{mole}\right) \times \left(\frac{charge}{electron}\right)$$

$$= (6.023 \times 10^{23}) \times (1.6 \times 10^{-19})$$

And got to the Nernst equation which gives the relationship between the potential difference between 2 points involving charges and so on and so forth; one in charge transport and the concentration of the ions at those 2 places.

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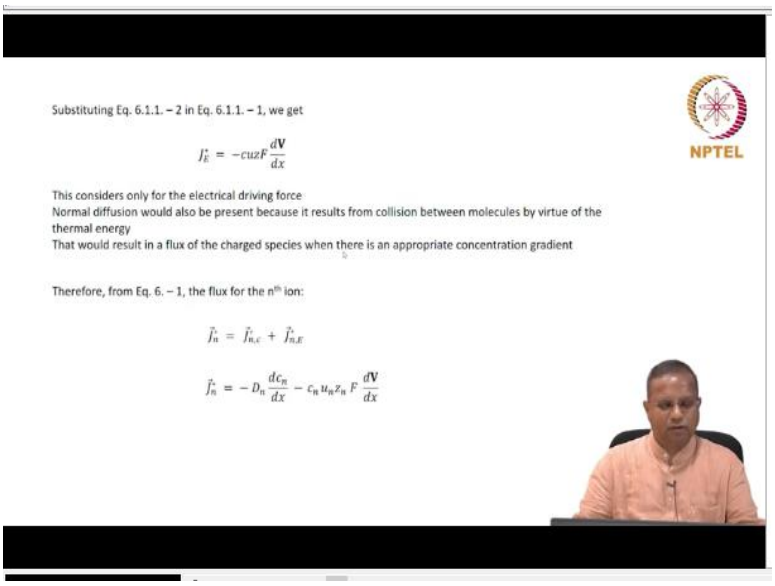

Substituting Eq. 6.1.1. – 2 in Eq. 6.1.1. – 1, we get

$$\vec{J}_E = -cuzF\frac{d\mathbf{V}}{dx}$$

This considers only for the electrical driving force
Normal diffusion would also be present because it results from collision between molecules by virtue of the thermal energy
That would result in a flux of the charged species when there is an appropriate concentration gradient

Therefore, from Eq. 6. – 1, the flux for the nth ion:

$$\vec{J}_n = \vec{J}_{n,c} + \vec{J}_{n,E}$$

$$\vec{J}_n = -D_n\frac{dc_n}{dx} - c_n u_n z_n F\frac{d\mathbf{V}}{dx}$$

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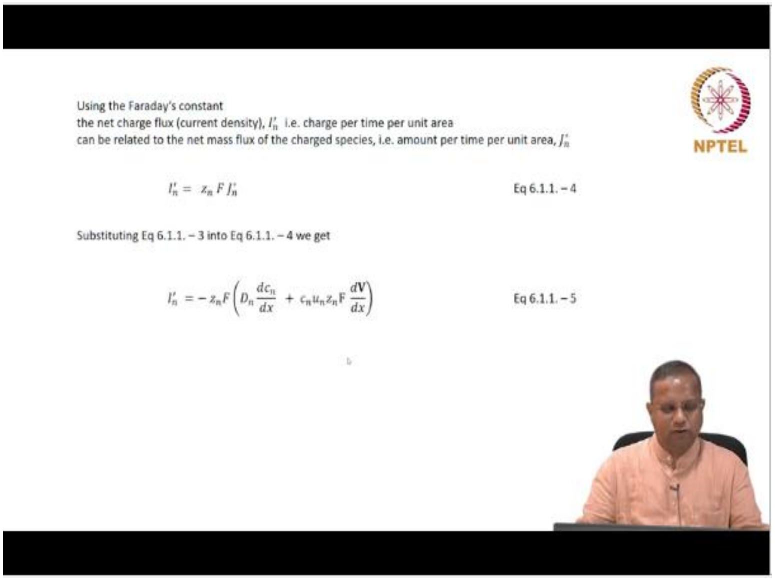

Using the Faraday's constant
the net charge flux (current density), I'_n i.e. charge per time per unit area
can be related to the net mass flux of the charged species, i.e. amount per time per unit area, J'_n

$$I'_n = z_n F J'_n \qquad \text{Eq 6.1.1.} - 4$$

Substituting Eq 6.1.1. – 3 into Eq 6.1.1. – 4 we get

$$I'_n = -z_n F\left(D_n \frac{dc_n}{dx} + c_n u_n z_n \mathrm{F} \frac{d\mathbf{V}}{dx}\right) \qquad \text{Eq 6.1.1.} - 5$$

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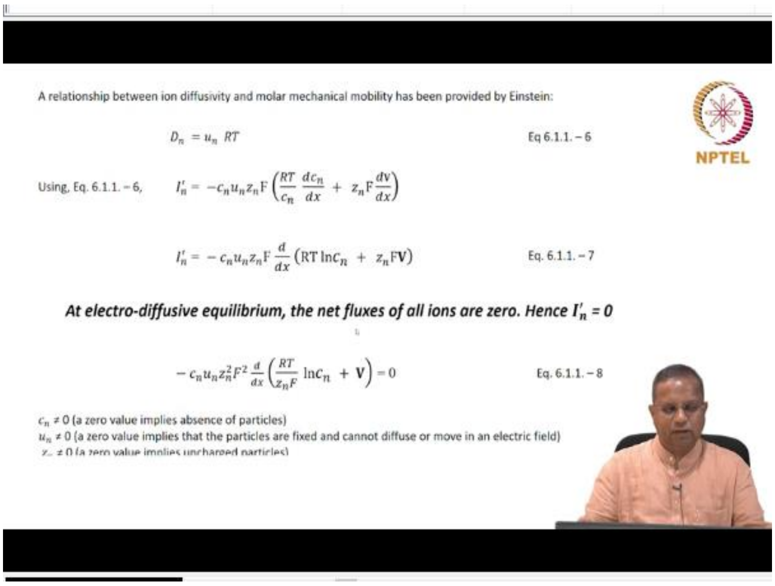

A relationship between ion diffusivity and molar mechanical mobility has been provided by Einstein:

$$D_n = u_n \, RT \qquad \text{Eq 6.1.1.} - 6$$

Using, Eq. 6.1.1. – 6, $I'_n = -c_n u_n z_n \mathrm{F}\left(\frac{RT}{c_n}\frac{dc_n}{dx} + z_n \mathrm{F}\frac{dv}{dx}\right)$

$$I'_n = -c_n u_n z_n \mathrm{F} \frac{d}{dx}\left(\mathrm{RT} \ln c_n + z_n \mathrm{F}\mathbf{V}\right) \qquad \text{Eq. 6.1.1.} - 7$$

At electro-diffusive equilibrium, the net fluxes of all ions are zero. Hence $I'_n = 0$

$$-c_n u_n z_n^2 F^2 \frac{d}{dx}\left(\frac{RT}{z_n F} \ln c_n + \mathbf{V}\right) = 0 \qquad \text{Eq. 6.1.1.} - 8$$

$c_n \neq 0$ (a zero value implies absence of particles)
$u_n \neq 0$ (a zero value implies that the particles are fixed and cannot diffuse or move in an electric field)
$z_n \neq 0$ (a zero value implies uncharged particles)

So, that was we looked at electro diffuser equilibrium on our way to the Nernst equation, the Einstein's relationship between the diffusivity and molar mobility.

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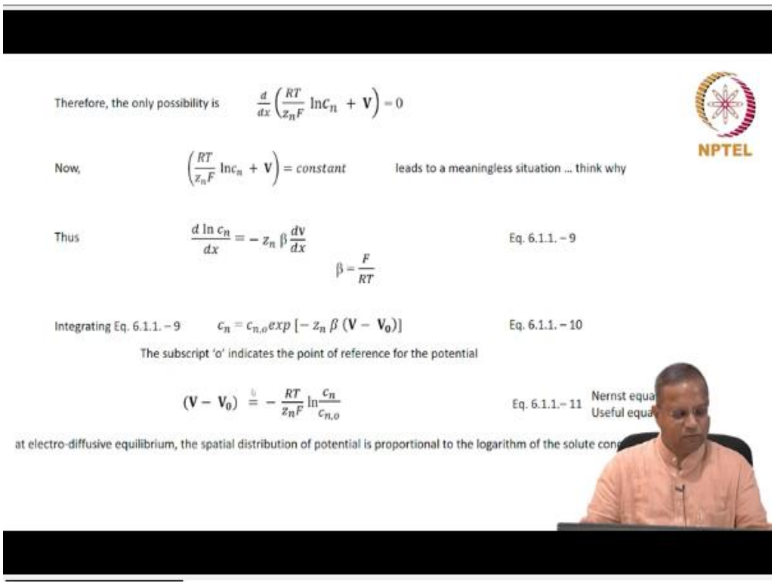

Therefore, the only possibility is $\frac{d}{dx}\left(\frac{RT}{z_n F}\ln c_n + \mathbf{V}\right) = 0$

Now, $\left(\frac{RT}{z_n F}\ln c_n + \mathbf{V}\right) = constant$ leads to a meaningless situation … think why

Thus $\frac{d \ln c_n}{dx} = - z_n \beta \frac{dv}{dx}$ Eq. 6.1.1. – 9

$\beta = \frac{F}{RT}$

Integrating Eq. 6.1.1. – 9 $c_n = c_{n,o} exp\left[- z_n \beta \left(\mathbf{V} - \mathbf{V_0}\right)\right]$ Eq. 6.1.1. – 10

The subscript 'o' indicates the point of reference for the potential

$(\mathbf{V} - \mathbf{V_0}) = - \frac{RT}{z_n F} \ln \frac{c_n}{c_{n,o}}$ Eq. 6.1.1.– 11 Nernst equa

Useful equa

at electro-diffusive equilibrium, the spatial distribution of potential is proportional to the logarithm of the solute con

And then the basis for our electric diffuser equilibrium then this was our Nernst equation okay. Nernst equation of course, is a very useful equation, we saw various applications of the Nernst equation, whenever there's a refusal equilibrium Nernst equation is better.

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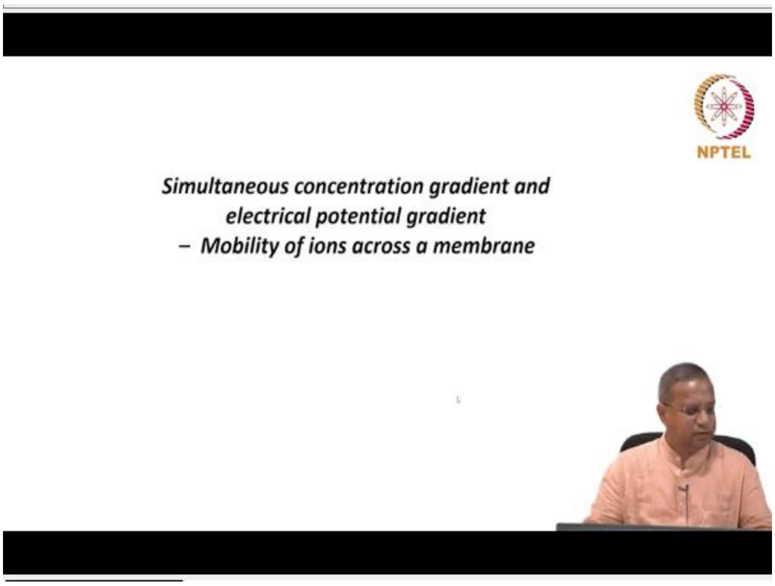

Simultaneous concentration gradient and electrical potential gradient – Mobility of ions across a membrane

So, then we saw the mobility of ions across a membrane, we saw how the Nernst equation could be used just the presence of a physical layer does not really matter, Nernst equation must be valid.

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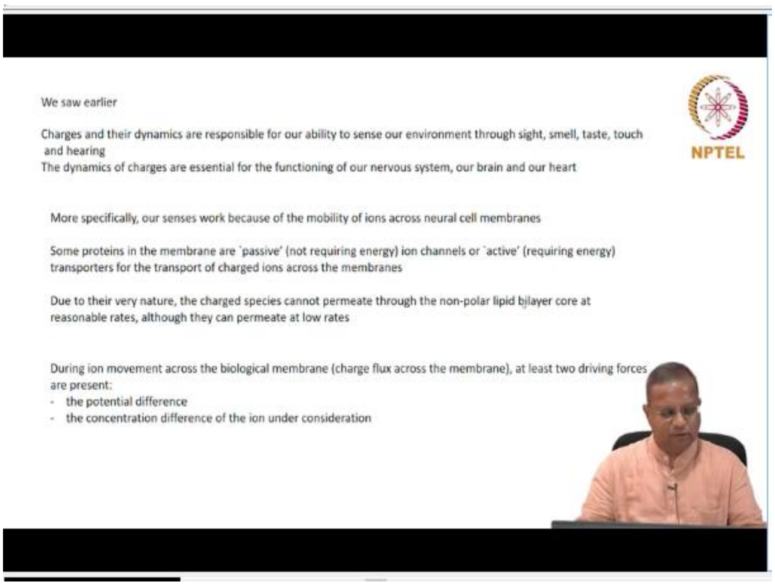

We saw earlier

Charges and their dynamics are responsible for our ability to sense our environment through sight, smell, taste, touch and hearing
The dynamics of charges are essential for the functioning of our nervous system, our brain and our heart

More specifically, our senses work because of the mobility of ions across neural cell membranes

Some proteins in the membrane are `passive' (not requiring energy) ion channels or `active' (requiring energy) transporters for the transport of charged ions across the membranes

Due to their very nature, the charged species cannot permeate through the non-polar lipid bilayer core at reasonable rates, although they can permeate at low rates

During ion movement across the biological membrane (charge flux across the membrane), at least two driving forces are present:
- the potential difference
- the concentration difference of the ion under consideration

However, in a real membrane, when you have multiple or even an any membrane may have multiple charges, distributing themselves at the same time as it happens in the case of neuronal membranes, that is the basis for our census to work and so on, so forth. Then we looked at some approximations that will work very well for analysis which is done in equilibrium approximation where the transports of individual ions are taken to be independent of each other.

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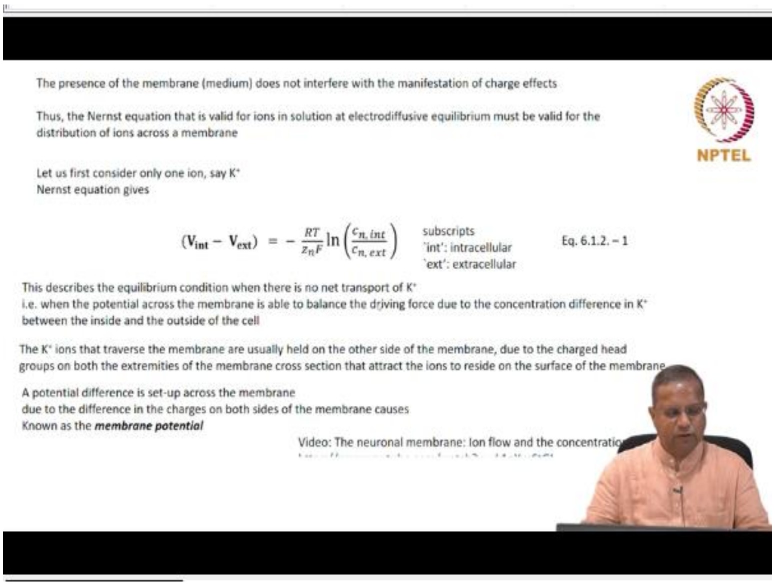

The presence of the membrane (medium) does not interfere with the manifestation of charge effects

Thus, the Nernst equation that is valid for ions in solution at electrodiffusive equilibrium must be valid for the distribution of ions across a membrane

Let us first consider only one ion, say K^+
Nernst equation gives

$$(\mathbf{V_{int}} - \mathbf{V_{ext}}) \;=\; -\frac{RT}{z_n F}\ln\left(\frac{c_{n,\,int}}{c_{n,\,ext}}\right) \qquad \text{Eq. 6.1.2.} - 1$$

subscripts
`int': intracellular
`ext': extracellular

This describes the equilibrium condition when there is no net transport of K^+
i.e. when the potential across the membrane is able to balance the driving force due to the concentration difference in K^+ between the inside and the outside of the cell

The K^+ ions that traverse the membrane are usually held on the other side of the membrane, due to the charged head groups on both the extremities of the membrane cross section that attract the ions to reside on the surface of the membrane

A potential difference is set-up across the membrane
due to the difference in the charges on both sides of the membrane causes
Known as the ***membrane potential***

Video: The neuronal membrane: Ion flow and the concentratio

So, then we got some useful relationships there, the membrane potential and so on.

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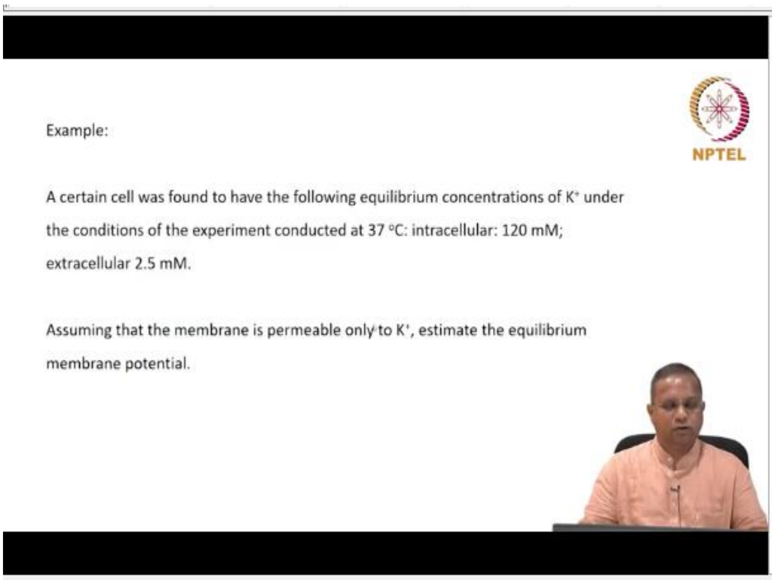

Example:

A certain cell was found to have the following equilibrium concentrations of K⁺ under the conditions of the experiment conducted at 37 °C: intracellular: 120 mM; extracellular 2.5 mM.

Assuming that the membrane is permeable only to K⁺, estimate the equilibrium membrane potential.

Then we worked out some examples also.

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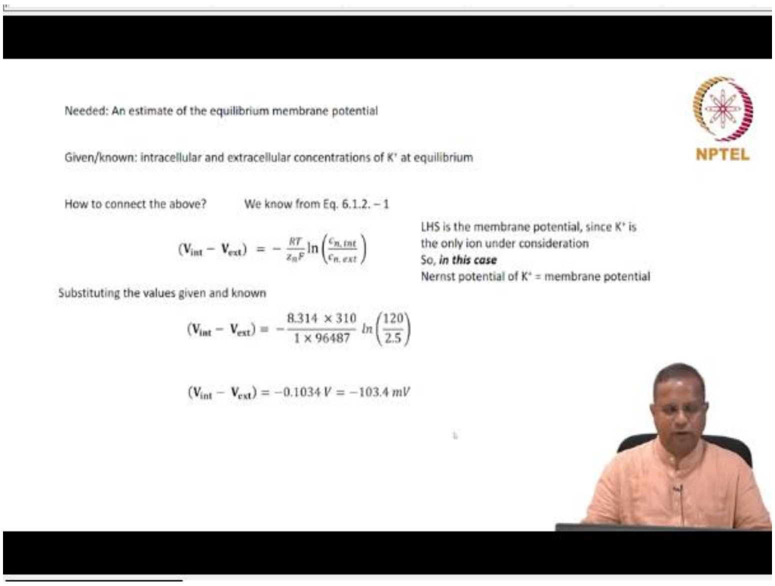

Needed: An estimate of the equilibrium membrane potential

Given/known: intracellular and extracellular concentrations of K⁺ at equilibrium

How to connect the above? We know from Eq. 6.1.2. – 1

$$(\mathbf{V_{int}} - \mathbf{V_{ext}}) = -\frac{RT}{z_n F}\ln\left(\frac{c_{n,int}}{c_{n,ext}}\right)$$

LHS is the membrane potential, since K⁺ is the only ion under consideration
So, ***in this case***
Nernst potential of K⁺ = membrane potential

Substituting the values given and known

$$(\mathbf{V_{int}} - \mathbf{V_{ext}}) = -\frac{8.314 \times 310}{1 \times 96487}\, ln\left(\frac{120}{2.5}\right)$$

$$(\mathbf{V_{int}} - \mathbf{V_{ext}}) = -0.1034\,V = -103.4\,mV$$

Very straightforward examples in this case.

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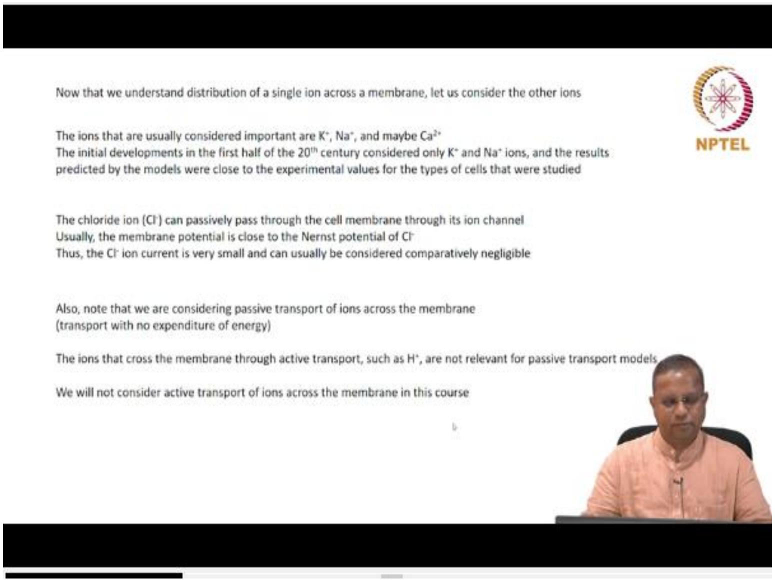

Now that we understand distribution of a single ion across a membrane, let us consider the other ions

The ions that are usually considered important are K^+, Na^+, and maybe Ca^{2+}
The initial developments in the first half of the 20th century considered only K^+ and Na^+ ions, and the results predicted by the models were close to the experimental values for the types of cells that were studied

The chloride ion (Cl^-) can passively pass through the cell membrane through its ion channel
Usually, the membrane potential is close to the Nernst potential of Cl^-
Thus, the Cl^- ion current is very small and can usually be considered comparatively negligible

Also, note that we are considering passive transport of ions across the membrane
(transport with no expenditure of energy)

The ions that cross the membrane through active transport, such as H^+, are not relevant for passive transport models

We will not consider active transport of ions across the membrane in this course

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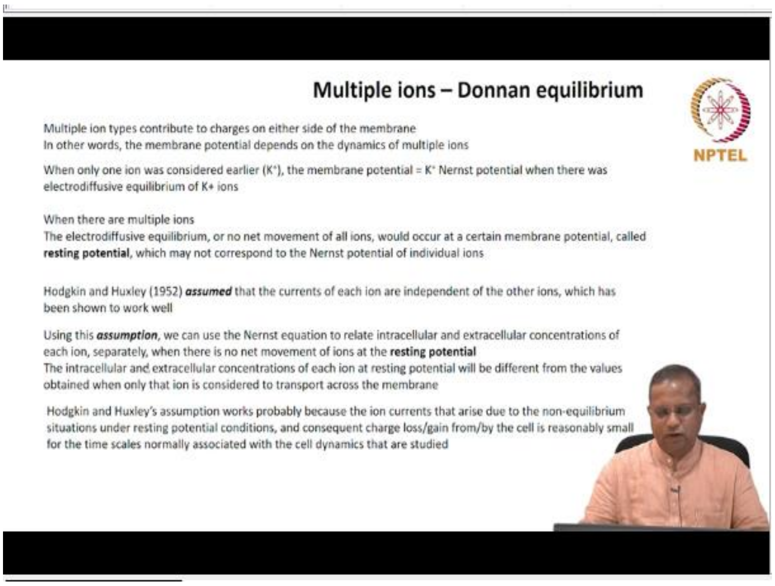

Multiple ions – Donnan equilibrium

Multiple ion types contribute to charges on either side of the membrane
In other words, the membrane potential depends on the dynamics of multiple ions

When only one ion was considered earlier (K^+), the membrane potential = K^+ Nernst potential when there was electrodiffusive equilibrium of K+ ions

When there are multiple ions
The electrodiffusive equilibrium, or no net movement of all ions, would occur at a certain membrane potential, called **resting potential**, which may not correspond to the Nernst potential of individual ions

Hodgkin and Huxley (1952) ***assumed*** that the currents of each ion are independent of the other ions, which has been shown to work well

Using this ***assumption***, we can use the Nernst equation to relate intracellular and extracellular concentrations of each ion, separately, when there is no net movement of ions at the **resting potential**
The intracellular and extracellular concentrations of each ion at resting potential will be different from the values obtained when only that ion is considered to transport across the membrane

Hodgkin and Huxley's assumption works probably because the ion currents that arise due to the non-equilibrium situations under resting potential conditions, and consequent charge loss/gain from/by the cell is reasonably small for the time scales normally associated with the cell dynamics that are studied

This is what Donnan equilibrium was multiple ion types, they distribute at the same time, then assume that the currents of each ion are independent of the other ions.

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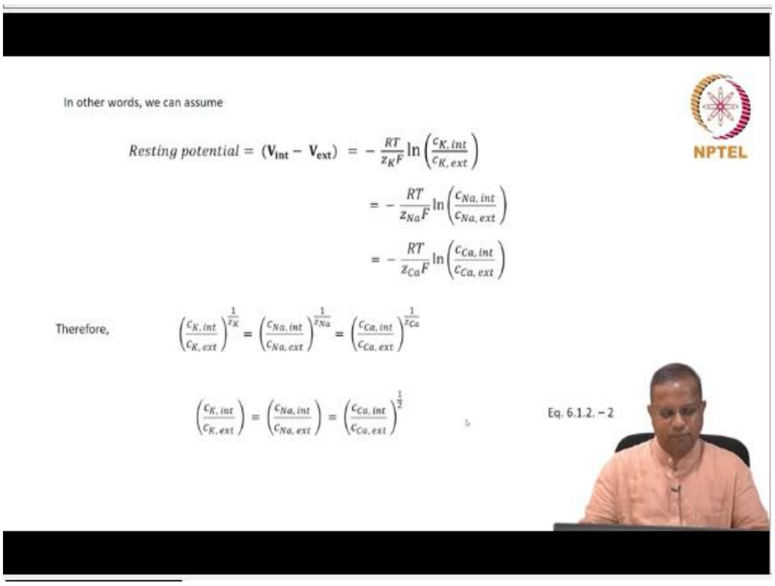

In other words, we can assume

$$\text{Resting potential} = (\mathbf{V}_{\mathbf{int}} - \mathbf{V}_{\mathbf{ext}}) = -\frac{RT}{z_K F}\ln\left(\frac{c_{K,\,int}}{c_{K,\,ext}}\right)$$

$$= -\frac{RT}{z_{Na} F}\ln\left(\frac{c_{Na,\,int}}{c_{Na,\,ext}}\right)$$

$$= -\frac{RT}{z_{Ca} F}\ln\left(\frac{c_{Ca,\,int}}{c_{Ca,\,ext}}\right)$$

Therefore,
$$\left(\frac{c_{K,\,int}}{c_{K,\,ext}}\right)^{\frac{1}{z_K}} = \left(\frac{c_{Na,\,int}}{c_{Na,\,ext}}\right)^{\frac{1}{z_{Na}}} = \left(\frac{c_{Ca,\,int}}{c_{Ca,\,ext}}\right)^{\frac{1}{z_{Ca}}}$$

$$\left(\frac{c_{K,\,int}}{c_{K,\,ext}}\right) = \left(\frac{c_{Na,\,int}}{c_{Na,\,ext}}\right) = \left(\frac{c_{Ca,\,int}}{c_{Ca,\,ext}}\right)^{\frac{1}{2}} \qquad \text{Eq. 6.1.2.} - 2$$

That is the basic idea. Then you could write the relationship between the ratios of these various ions at equilibrium.

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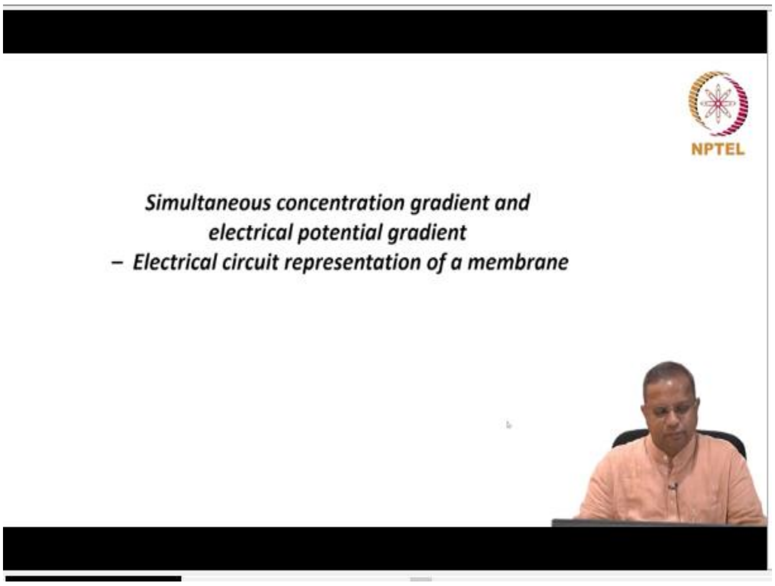

Simultaneous concentration gradient and electrical potential gradient
– Electrical circuit representation of a membrane

The membrane potential ideas we saw there. Then, we looked at the electrical circuit representation of a membrane, we said that the membrane consists of the lipid bilayer, which is nothing but charges separated by the lipid part which can be considered a dielectric. Therefore, that is a typical capacitor and then the ion channels which cause the passive flux of ions across them.

Active transport as not a part of our models; not a part of a concentration in this course. So, the passive transport can be modeled as resistance and the Nernst potential combination and so on and so forth. Then let me at least briefly show you what those, what the representation looks like. Yeah.

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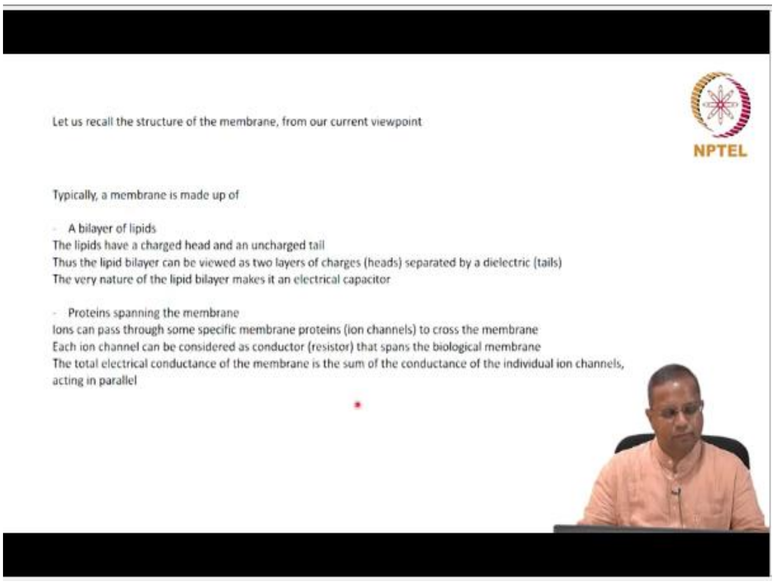

Let us recall the structure of the membrane, from our current viewpoint

Typically, a membrane is made up of

- A bilayer of lipids

The lipids have a charged head and an uncharged tail
Thus the lipid bilayer can be viewed as two layers of charges (heads) separated by a dielectric (tails)
The very nature of the lipid bilayer makes it an electrical capacitor

- Proteins spanning the membrane

Ions can pass through some specific membrane proteins (ion channels) to cross the membrane
Each ion channel can be considered as conductor (resistor) that spans the biological membrane
The total electrical conductance of the membrane is the sum of the conductance of the individual ion channels, acting in parallel

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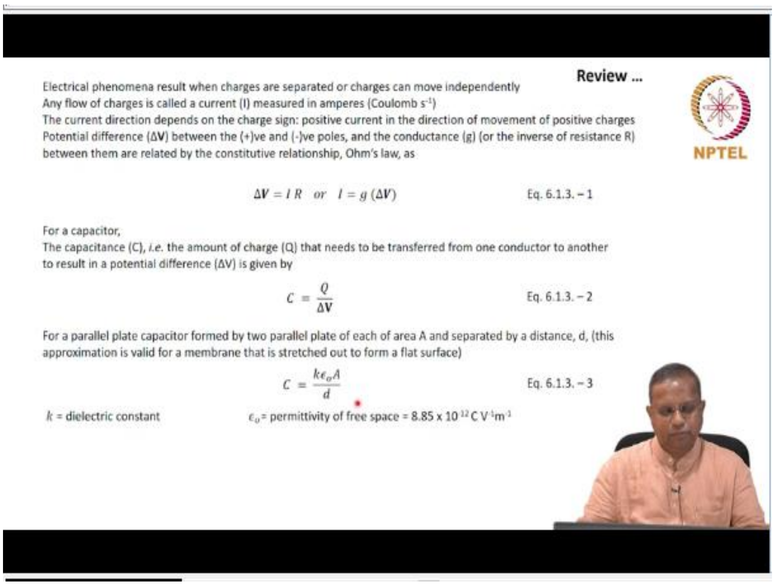

Review ...

Electrical phenomena result when charges are separated or charges can move independently
Any flow of charges is called a current (I) measured in amperes (Coulomb s^{-1})
The current direction depends on the charge sign: positive current in the direction of movement of positive charges
Potential difference (ΔV) between the (+)ve and (-)ve poles, and the conductance (g) (or the inverse of resistance R) between them are related by the constitutive relationship, Ohm's law, as

$$\Delta V = I\,R \quad or \quad I = g\,(\Delta V) \qquad \text{Eq. 6.1.3.} - 1$$

For a capacitor,
The capacitance (C), *i.e.* the amount of charge (Q) that needs to be transferred from one conductor to another to result in a potential difference (ΔV) is given by

$$C = \frac{Q}{\Delta V} \qquad \text{Eq. 6.1.3.} - 2$$

For a parallel plate capacitor formed by two parallel plate of each of area A and separated by a distance, d, (this approximation is valid for a membrane that is stretched out to form a flat surface)

$$C = \frac{k\epsilon_o A}{d} \qquad \text{Eq. 6.1.3.} - 3$$

k = dielectric constant

ϵ_o = permittivity of free space = $8.85 \times 10^{-12}\ C\,V^{-1}m^{-1}$

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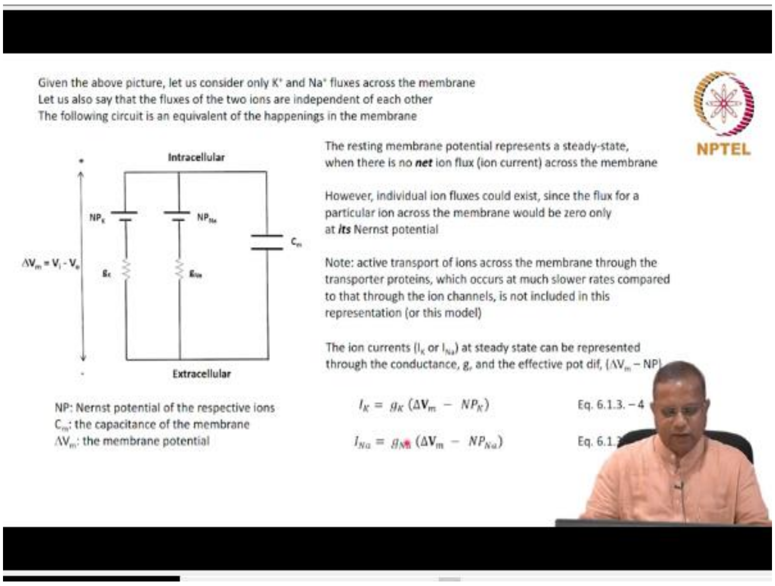
Given the above picture, let us consider only K^+ and Na^+ fluxes across the membrane
Let us also say that the fluxes of the two ions are independent of each other
The following circuit is an equivalent of the happenings in the membrane

The resting membrane potential represents a steady-state, when there is no ***net*** ion flux (ion current) across the membrane

However, individual ion fluxes could exist, since the flux for a particular ion across the membrane would be zero only at ***its*** Nernst potential

Note: active transport of ions across the membrane through the transporter proteins, which occurs at much slower rates compared to that through the ion channels, is not included in this representation (or this model)

The ion currents (I_K or I_{Na}) at steady state can be represented through the conductance, g, and the effective pot dif, (ΔV_m – NP)

NP: Nernst potential of the respective ions
C_m: the capacitance of the membrane
ΔV_m: the membrane potential

$$I_K = g_K\,(\Delta \mathbf{V}_m - NP_K) \qquad \text{Eq. 6.1.3.} - 4$$

$$I_{Na} = g_{Na}\,(\Delta \mathbf{V}_m - NP_{Na}) \qquad \text{Eq. 6.1.}$$

So, the membrane has been converted into its electrical equivalent. So, you could apply electrical principles to analyze it. So, this is the lipid bilayer membrane a capacitance, this is the ion channel for sodium. So, this is the conductance of the ion channel and a Nernst potential for sodium conductance of the potassium channel and Nernst potential for potassium, the intracellular part, the extracellular part, intercellular minus extracellular is taken as the membrane potential $\Delta V_m = V_i - V_o$. We had seen this and then we worked out some relationships between the ionic currents.

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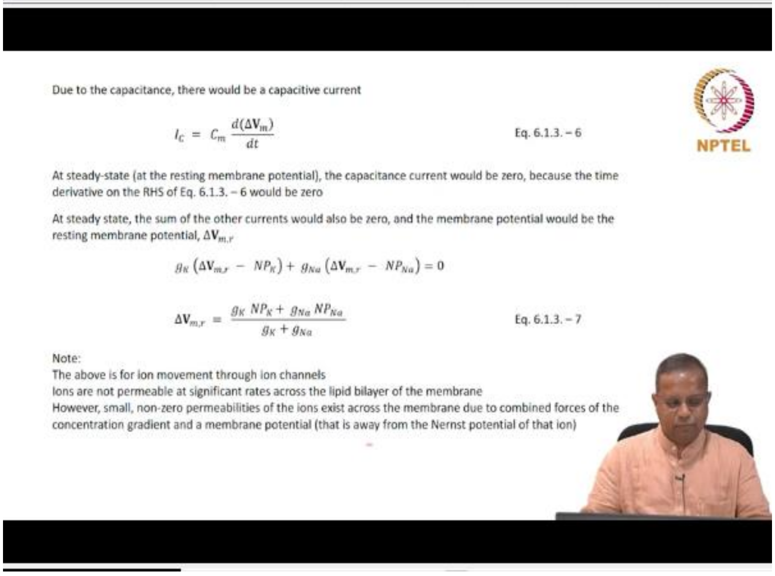
Due to the capacitance, there would be a capacitive current

$$I_C = C_m \frac{d(\Delta \mathbf{V}_m)}{dt} \qquad \text{Eq. 6.1.3.} - 6$$

At steady-state (at the resting membrane potential), the capacitance current would be zero, because the time derivative on the RHS of Eq. 6.1.3. – 6 would be zero

At steady state, the sum of the other currents would also be zero, and the membrane potential would be the resting membrane potential, $\Delta \mathbf{V}_{m,r}$

$$g_K\left(\Delta \mathbf{V}_{m,r} - NP_K\right) + g_{Na}\left(\Delta \mathbf{V}_{m,r} - NP_{Na}\right) = 0$$

$$\Delta \mathbf{V}_{m,r} = \frac{g_K\,NP_K + g_{Na}\,NP_{Na}}{g_K + g_{Na}} \qquad \text{Eq. 6.1.3.} - 7$$

Note:
The above is for ion movement through ion channels
Ions are not permeable at significant rates across the lipid bilayer of the membrane
However, small, non-zero permeabilities of the ions exist across the membrane due to combined forces of the concentration gradient and a membrane potential (that is away from the Nernst potential of that ion)

And the membrane potential and so on so forth okay. This was the resting membrane potential, ion currents Nernst potentials of the ions, if only potassium and sodium are involved excuse me.

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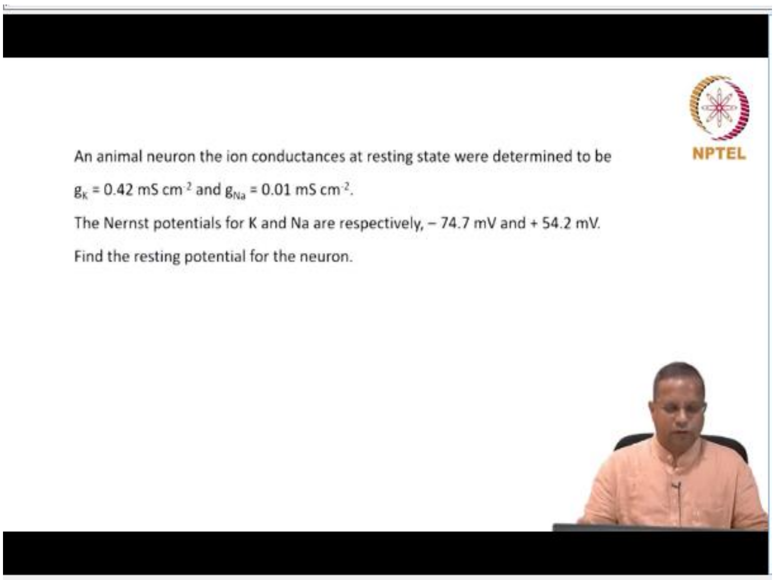

An animal neuron the ion conductances at resting state were determined to be

$g_K = 0.42$ mS cm^{-2} and $g_{Na} = 0.01$ mS cm^{-2}.

The Nernst potentials for K and Na are respectively, – 74.7 mV and + 54.2 mV.

Find the resting potential for the neuron.

We also worked on some examples there. Then we looked at the action potential which forms the basis for all our senses, it is nothing but the dynamics of the ion transport across a neuronal membrane, as we look at sodium and potassium alone, and that is good enough for most situations, bring calcium at times and so on, so forth. So, we looked at the basis for action potential.

And how a series of action potential and potentials can arise in a very short time of a few microseconds across the entire length of the neuron and that results in the axial current. That is how we are able to sense or react. Then we applied or showed the applications of these principles to electrophoresis which is an important process either in the lab or in the industry, electro focusing is an important process in the industry, the principles were shown.

So, this is what we did for the situation where there is a concentration gradient and an electrical potential gradient at the same time, okay, very many applications, some fundamental aspects we had covered there.

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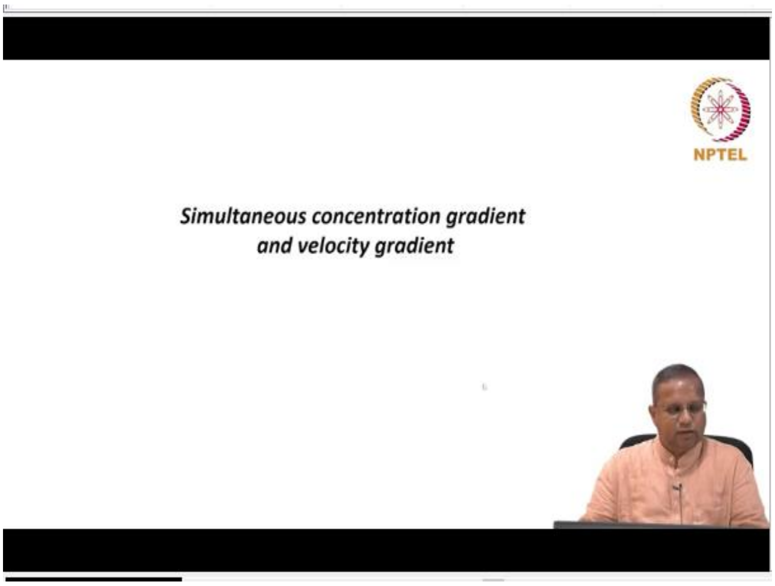

Simultaneous concentration gradient and velocity gradient

Then when we looked at simultaneous concentration gradient and velocity gradient.

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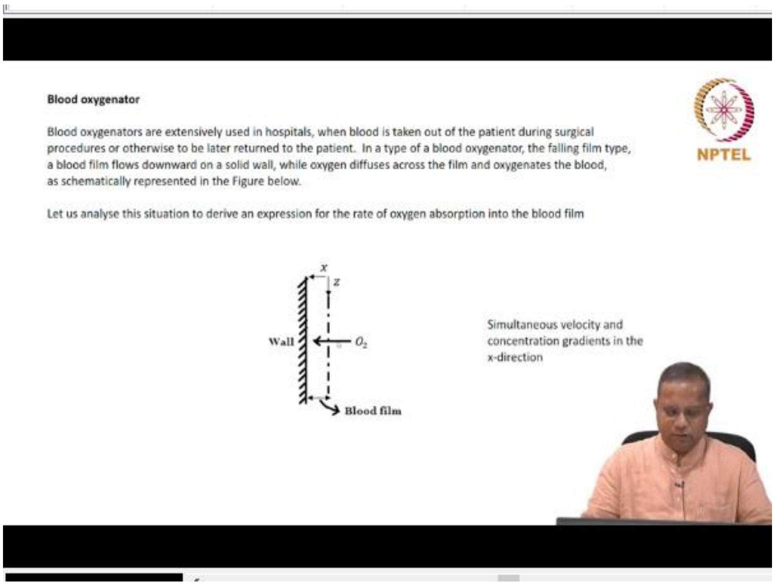

Blood oxygenator

Blood oxygenators are extensively used in hospitals, when blood is taken out of the patient during surgical procedures or otherwise to be later returned to the patient. In a type of a blood oxygenator, the falling film type, a blood film flows downward on a solid wall, while oxygen diffuses across the film and oxygenates the blood, as schematically represented in the Figure below.

Let us analyse this situation to derive an expression for the rate of oxygen absorption into the blood film

Simultaneous velocity and concentration gradients in the x-direction

Here, we looked at the case of the blood oxygenated where there is a thin layer of blood that flows and oxygen from the air oxygenates the blood that goes through the blood oxygenated. Of course, all this is kept in a sterile box and so on and so forth. We analyze the situation here, through an equations approach.

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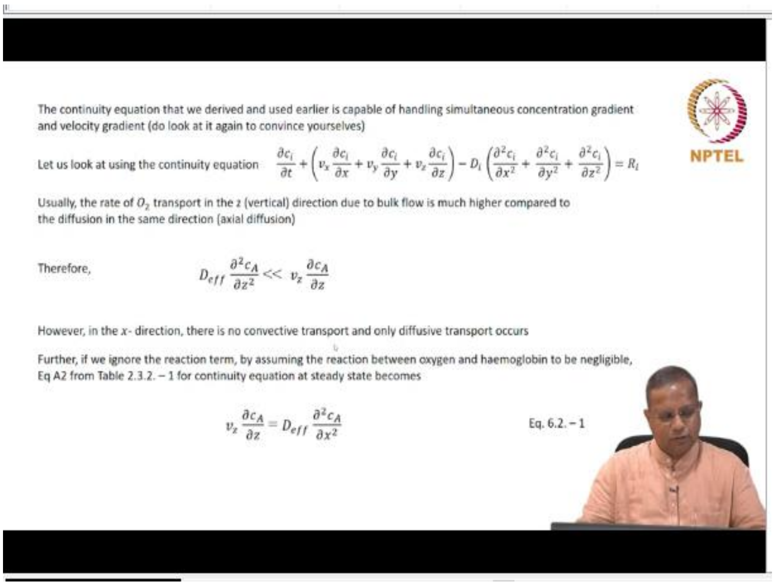

The continuity equation that we derived and used earlier is capable of handling simultaneous concentration gradient and velocity gradient (do look at it again to convince yourselves)

Let us look at using the continuity equation $\frac{\partial c_i}{\partial t} + \left(v_x \frac{\partial c_i}{\partial x} + v_y \frac{\partial c_i}{\partial y} + v_z \frac{\partial c_i}{\partial z} \right) - D_i \left(\frac{\partial^2 c_i}{\partial x^2} + \frac{\partial^2 c_i}{\partial y^2} + \frac{\partial^2 c_i}{\partial z^2} \right) = R_i$

Usually, the rate of O_2 transport in the z (vertical) direction due to bulk flow is much higher compared to the diffusion in the same direction (axial diffusion)

Therefore, $D_{eff} \frac{\partial^2 c_A}{\partial z^2} << v_z \frac{\partial c_A}{\partial z}$

However, in the x- direction, there is no convective transport and only diffusive transport occurs

Further, if we ignore the reaction term, by assuming the reaction between oxygen and haemoglobin to be negligible, Eq A2 from Table 2.3.2. – 1 for continuity equation at steady state becomes

$$v_z \frac{\partial c_A}{\partial z} = D_{eff} \frac{\partial^2 c_A}{\partial x^2} \qquad \text{Eq. 6.2.} - 1$$

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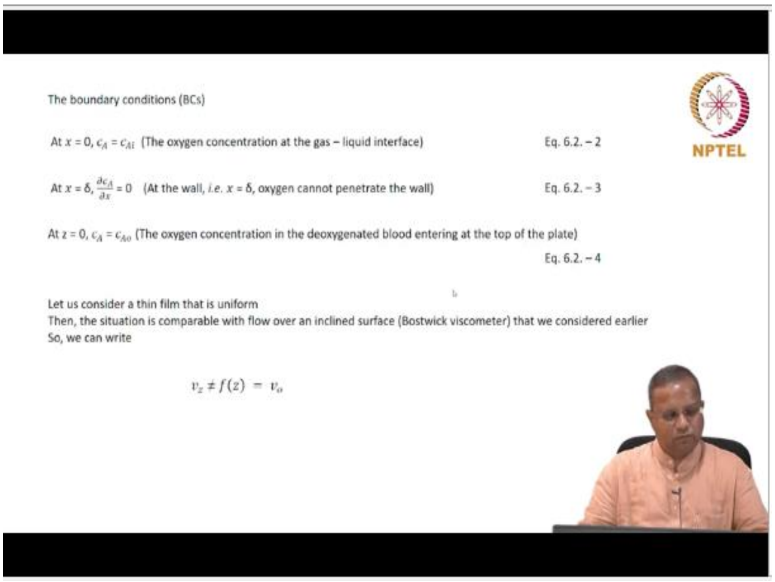

The boundary conditions (BCs)

At $x = 0$, $c_A = c_{Ai}$ (The oxygen concentration at the gas – liquid interface) Eq. 6.2. – 2

At $x = \delta$, $\frac{\partial c_A}{\partial x} = 0$ (At the wall, *i.e.* $x = \delta$, oxygen cannot penetrate the wall) Eq. 6.2. – 3

At $z = 0$, $c_A = c_{Ao}$ (The oxygen concentration in the deoxygenated blood entering at the top of the plate)
Eq. 6.2. – 4

Let us consider a thin film that is uniform
Then, the situation is comparable with flow over an inclined surface (Bostwick viscometer) that we considered earlier
So, we can write

$$v_z \neq f(z) = v_o$$

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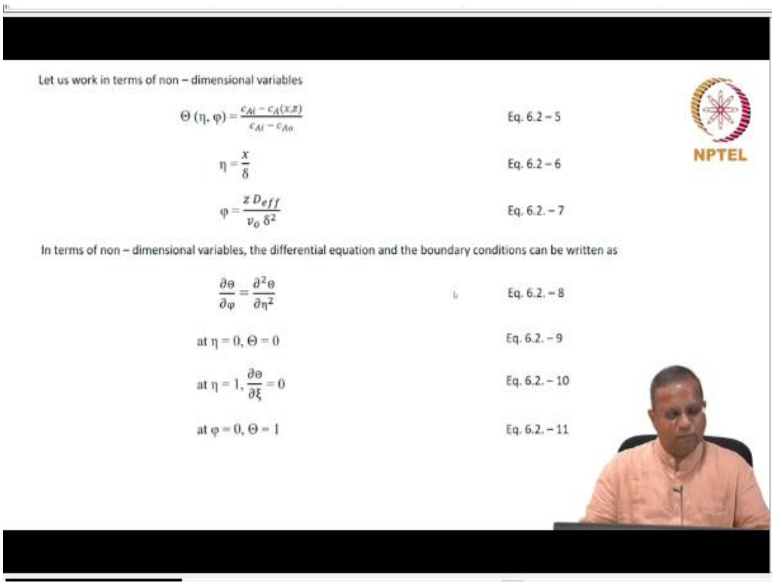

Let us work in terms of non – dimensional variables

$$\Theta(\eta, \varphi) = \frac{c_{Ai} - c_A(x,z)}{c_{Ai} - c_{Ao}} \qquad \text{Eq. 6.2 – 5}$$

$$\eta = \frac{x}{\delta} \qquad \text{Eq. 6.2 – 6}$$

$$\varphi = \frac{z\, D_{eff}}{v_o\, \delta^2} \qquad \text{Eq. 6.2. – 7}$$

In terms of non – dimensional variables, the differential equation and the boundary conditions can be written as

$$\frac{\partial \Theta}{\partial \varphi} = \frac{\partial^2 \Theta}{\partial \eta^2} \qquad \text{Eq. 6.2. – 8}$$

$$\text{at } \eta = 0, \Theta = 0 \qquad \text{Eq. 6.2. – 9}$$

$$\text{at } \eta = 1, \frac{\partial \Theta}{\partial \xi} = 0 \qquad \text{Eq. 6.2. – 10}$$

$$\text{at } \varphi = 0, \Theta = 1 \qquad \text{Eq. 6.2. – 11}$$

And I had also use this to tell you something about modeling itself right, I think.

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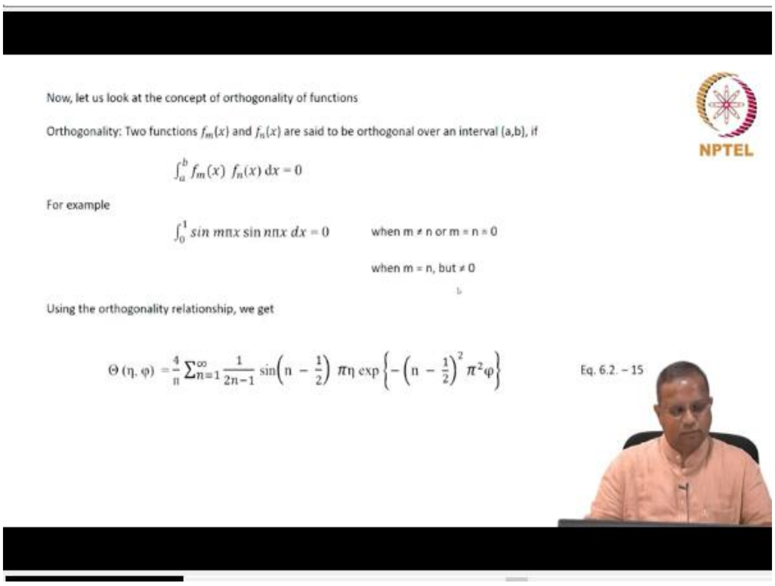

Now, let us look at the concept of orthogonality of functions

Orthogonality: Two functions $f_m(x)$ and $f_n(x)$ are said to be orthogonal over an interval (a,b), if

$$\int_a^b f_m(x)\, f_n(x)\, dx = 0$$

For example

$$\int_0^1 \sin m\pi x \sin n\pi x\, dx = 0 \qquad \text{when } m \neq n \text{ or } m = n = 0$$

$$\text{when } m = n, \text{ but } \neq 0$$

Using the orthogonality relationship, we get

$$\Theta(\eta, \varphi) = \frac{4}{\pi} \sum_{n=1}^{\infty} \frac{1}{2n-1} \sin\left(n - \frac{1}{2}\right) \pi\eta \exp\left\{-\left(n - \frac{1}{2}\right)^2 \pi^2 \varphi\right\} \qquad \text{Eq. 6.2. – 15}$$

This was the example that I had used.

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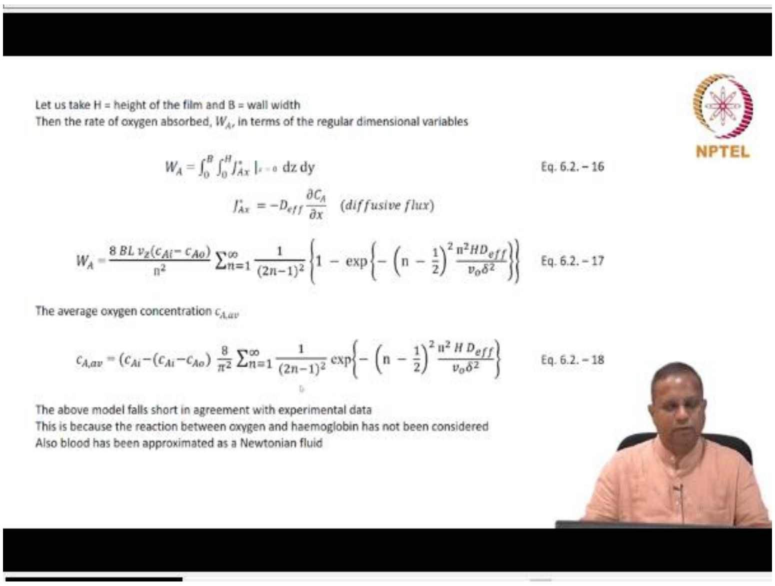

Let us take H = height of the film and B = wall width

Then the rate of oxygen absorbed, W_A, in terms of the regular dimensional variables

$$W_A = \int_0^B \int_0^H J^*_{Ax} |_{x=0}\, dz\, dy \qquad \text{Eq. 6.2.-16}$$

$$J^*_{Ax} = -D_{eff} \frac{\partial C_A}{\partial x} \quad (diffusive\ flux)$$

$$W_A = \frac{8\, BL\, v_z(c_{Ai} - c_{Ao})}{n^2} \sum_{n=1}^{\infty} \frac{1}{(2n-1)^2} \left\{1 - \exp\left\{-\left(n - \frac{1}{2}\right)^2 \frac{n^2 H D_{eff}}{v_0 \delta^2}\right\}\right\} \qquad \text{Eq. 6.2.-17}$$

The average oxygen concentration $c_{A,av}$

$$c_{A,av} = (c_{Ai} - (c_{Ai} - c_{Ao})\, \frac{8}{\pi^2} \sum_{n=1}^{\infty} \frac{1}{(2n-1)^2} \exp\left\{-\left(n - \frac{1}{2}\right)^2 \frac{n^2\, H\, D_{eff}}{v_0 \delta^2}\right\} \qquad \text{Eq. 6.2.-18}$$

The above model falls short in agreement with experimental data

This is because the reaction between oxygen and haemoglobin has not been considered

Also blood has been approximated as a Newtonian fluid

Yeah. The above model falls short in agreement with experimental data right. So, this is essentially the way the modeling was, modeled is a representation of course, we cannot represent everything. So, we represent these salient features of the physical system that is tested by testing the model presence against experimental data. If it is good fine, we are happy that we have captured the essential aspects of the system through the model.

Otherwise, we need to go back and refine the model. In this case some of the reasons why this is happening the disagreement is happening. Could be because the reaction between oxygen and hemoglobin has not been considered as well as the fact that the blood has been approximated as a Newtonian fluid right. So, this is an important aspect that you need to pick up for any mathematical modeling.

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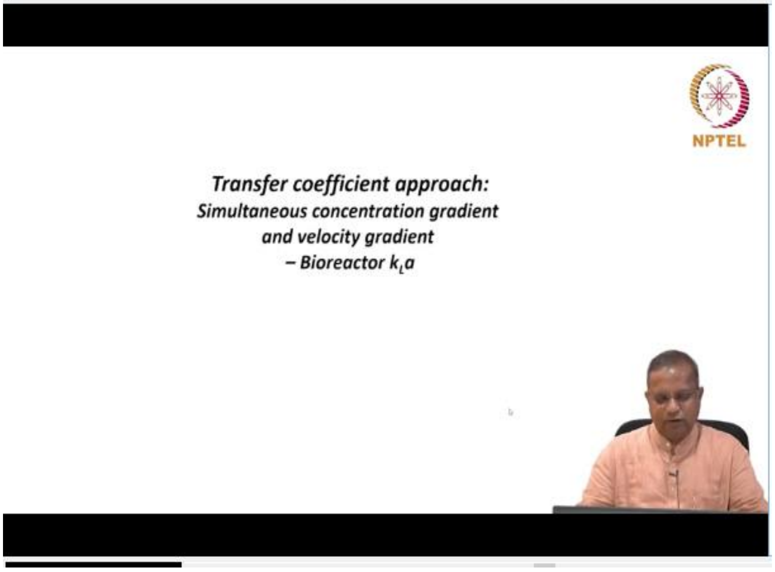

Transfer coefficient approach:
Simultaneous concentration gradient
and velocity gradient
– Bioreactor k_La

Then we delved into the transfer coefficient approach. First for the case of simultaneous concentration gradient and velocity gradient. We spent a good amount of time on the bioreactor k_La, which is the oxygen transfer ability of the bioreactor in this case of a bio system, which is something like this.

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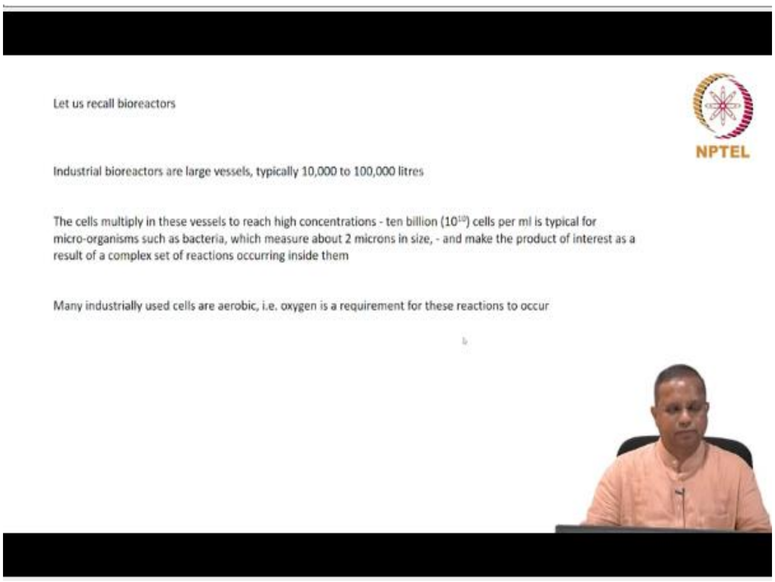

Let us recall bioreactors

Industrial bioreactors are large vessels, typically 10,000 to 100,000 litres

The cells multiply in these vessels to reach high concentrations - ten billion (10^{10}) cells per ml is typical for micro-organisms such as bacteria, which measure about 2 microns in size, - and make the product of interest as a result of a complex set of reactions occurring inside them

Many industrially used cells are aerobic, i.e. oxygen is a requirement for these reactions to occur

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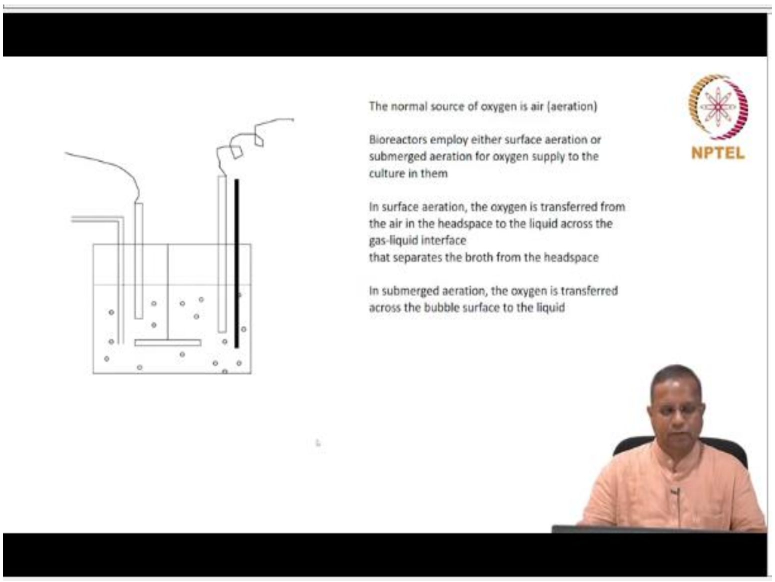

The normal source of oxygen is air (aeration)

Bioreactors employ either surface aeration or submerged aeration for oxygen supply to the culture in them

In surface aeration, the oxygen is transferred from the air in the headspace to the liquid across the gas-liquid interface that separates the broth from the headspace

In submerged aeration, the oxygen is transferred across the bubble surface to the liquid

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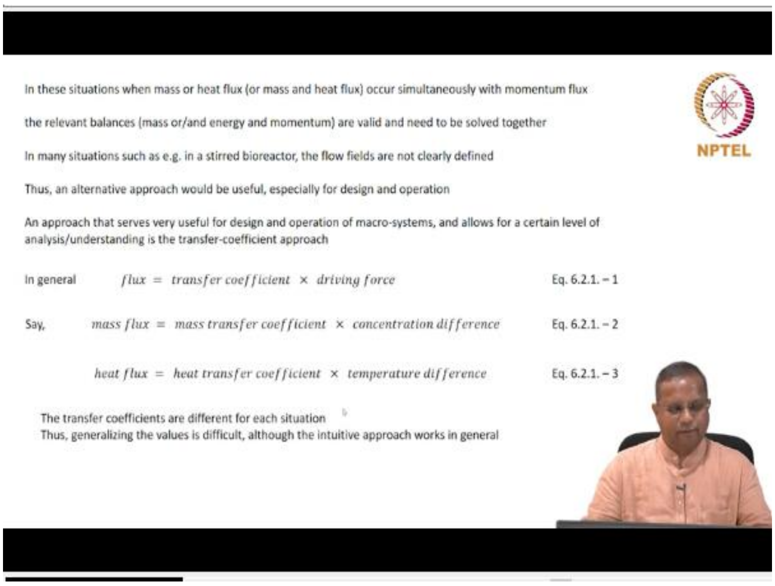

In these situations when mass or heat flux (or mass and heat flux) occur simultaneously with momentum flux

the relevant balances (mass or/and energy and momentum) are valid and need to be solved together

In many situations such as e.g. in a stirred bioreactor, the flow fields are not clearly defined

Thus, an alternative approach would be useful, especially for design and operation

An approach that serves very useful for design and operation of macro-systems, and allows for a certain level of analysis/understanding is the transfer-coefficient approach

In general $flux = transfer\ coefficient \times driving\ force$ Eq. 6.2.1. – 1

Say, $mass\ flux = mass\ transfer\ coefficient \times concentration\ difference$ Eq. 6.2.1. – 2

$heat\ flux = heat\ transfer\ coefficient \times temperature\ difference$ Eq. 6.2.1. – 3

The transfer coefficients are different for each situation
Thus, generalizing the values is difficult, although the intuitive approach works in general

That is a bioreactor there. So, we are using this approach here, mass flux sequence, mass transfer coefficient times the concentration difference.

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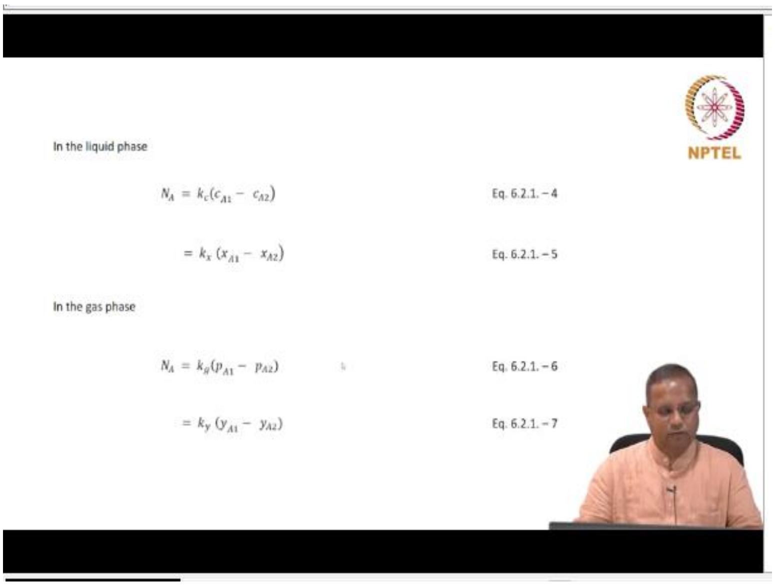

In the liquid phase

$$N_A = k_c(c_{A1} - c_{A2}) \quad \text{Eq. 6.2.1. – 4}$$

$$= k_x\,(x_{A1} - x_{A2}) \quad \text{Eq. 6.2.1. – 5}$$

In the gas phase

$$N_A = k_g(p_{A1} - p_{A2}) \quad \text{Eq. 6.2.1. – 6}$$

$$= k_y\,(y_{A1} - y_{A2}) \quad \text{Eq. 6.2.1. – 7}$$

And then we elaborately derived the case of transport from the gas phase to the liquid phase.

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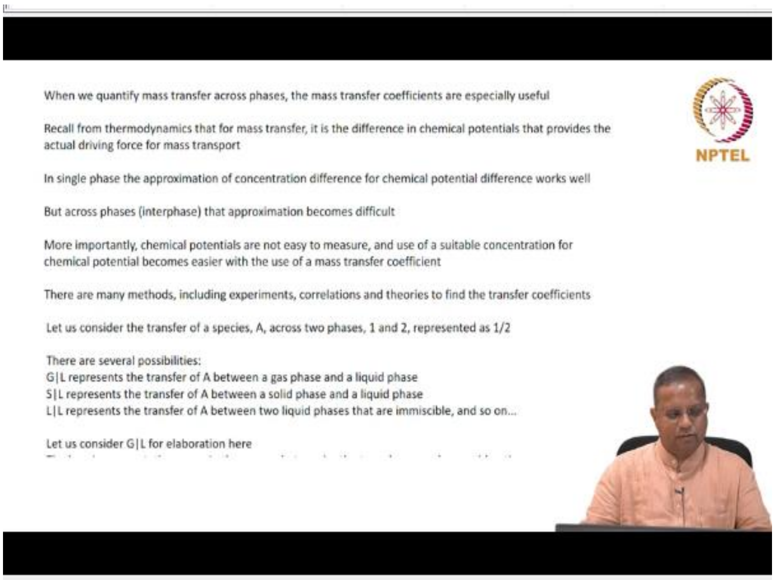

When we quantify mass transfer across phases, the mass transfer coefficients are especially useful

Recall from thermodynamics that for mass transfer, it is the difference in chemical potentials that provides the actual driving force for mass transport

In single phase the approximation of concentration difference for chemical potential difference works well

But across phases (interphase) that approximation becomes difficult

More importantly, chemical potentials are not easy to measure, and use of a suitable concentration for chemical potential becomes easier with the use of a mass transfer coefficient

There are many methods, including experiments, correlations and theories to find the transfer coefficients

Let us consider the transfer of a species, A, across two phases, 1 and 2, represented as 1/2

There are several possibilities:
G|L represents the transfer of A between a gas phase and a liquid phase
S|L represents the transfer of A between a solid phase and a liquid phase
L|L represents the transfer of A between two liquid phases that are immiscible, and so on...

Let us consider G|L for elaboration here

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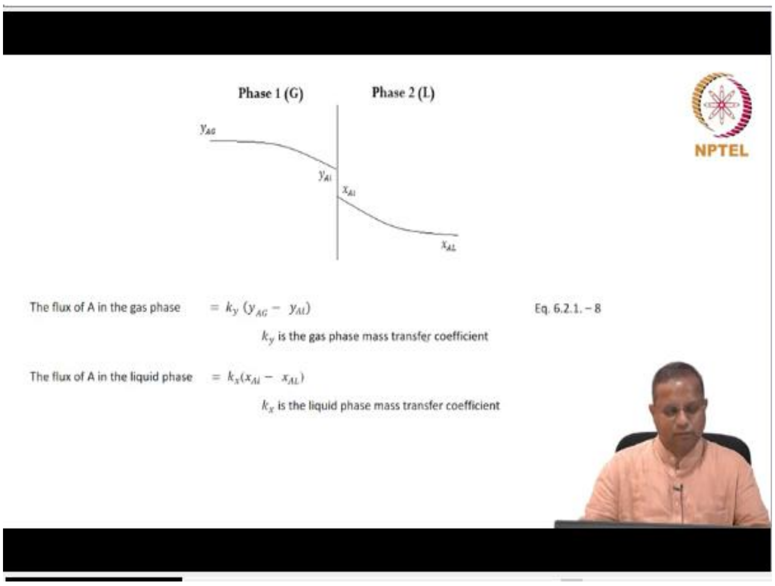

The flux of A in the gas phase $= k_y\,(y_{AG} - y_{Ai})$ Eq. 6.2.1. – 8

k_y is the gas phase mass transfer coefficient

The flux of A in the liquid phase $= k_x(x_{Ai} - x_{AL})$

k_x is the liquid phase mass transfer coefficient

The phase 1, phase 2, gas and liquid.

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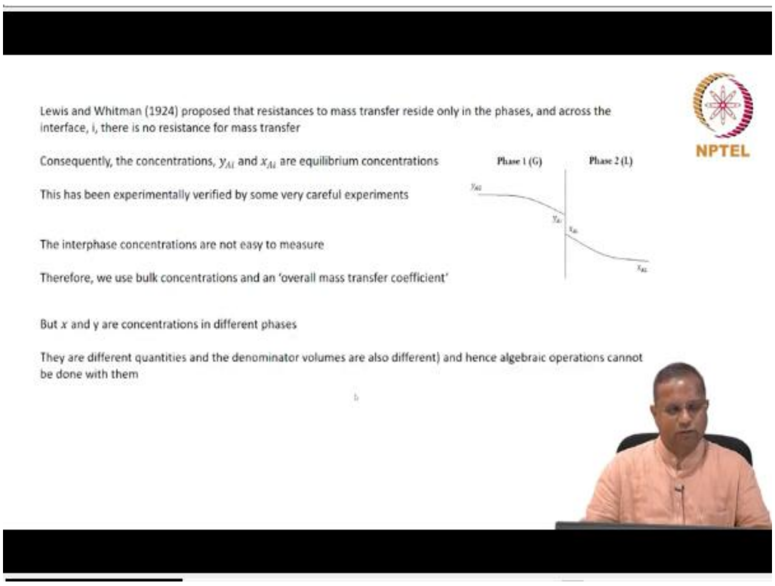

Lewis and Whitman (1924) proposed that resistances to mass transfer reside only in the phases, and across the interface, i, there is no resistance for mass transfer

Consequently, the concentrations, y_{Ai} and x_{Ai} are equilibrium concentrations

This has been experimentally verified by some very careful experiments

The interphase concentrations are not easy to measure

Therefore, we use bulk concentrations and an 'overall mass transfer coefficient'

But x and y are concentrations in different phases

They are different quantities and the denominator volumes are also different) and hence algebraic operations cannot be done with them

In our derivation here.

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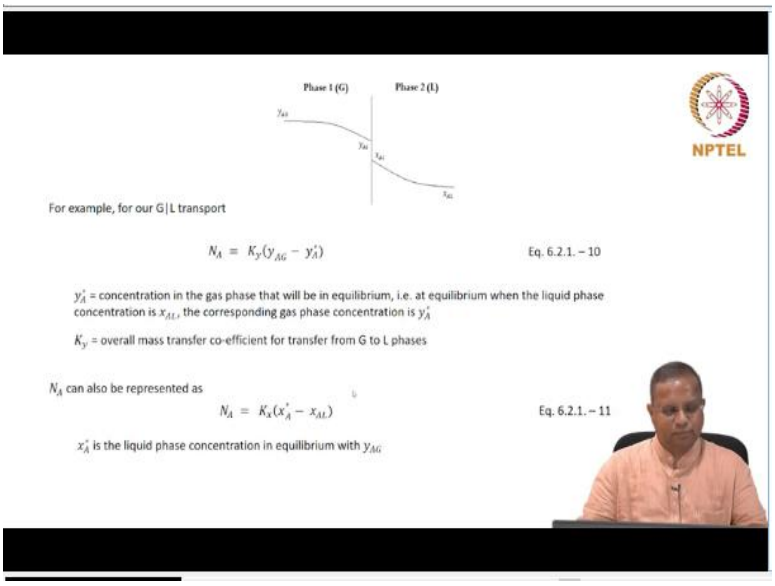

For example, for our G|L transport

$$N_A = K_y(y_{AG} - y_A^*) \qquad \text{Eq. 6.2.1.} - 10$$

y_A^* = concentration in the gas phase that will be in equilibrium, i.e. at equilibrium when the liquid phase concentration is x_{AL}, the corresponding gas phase concentration is y_A^*

K_y = overall mass transfer co-efficient for transfer from G to L phases

N_A can also be represented as

$$N_A = K_x(x_A^* - x_{AL}) \qquad \text{Eq. 6.2.1.} - 11$$

x_A^* is the liquid phase concentration in equilibrium with y_{AG}

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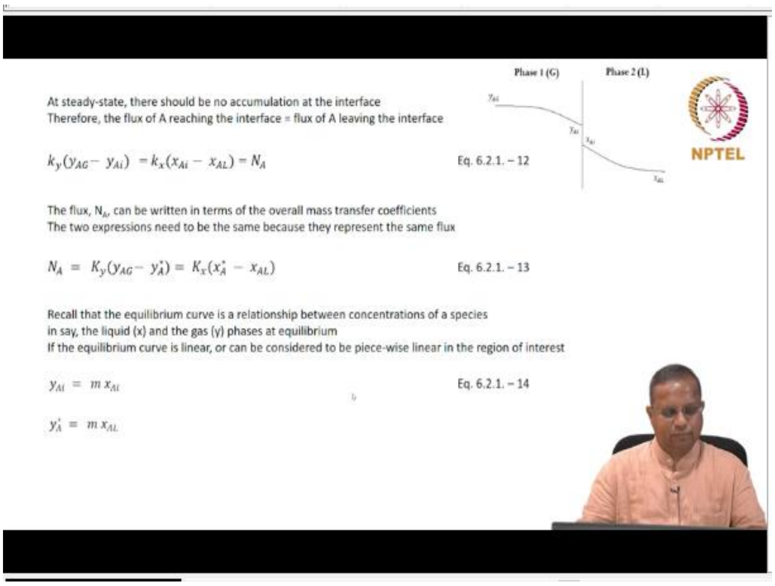

At steady-state, there should be no accumulation at the interface
Therefore, the flux of A reaching the interface = flux of A leaving the interface

$$k_y(y_{AG} - y_{Ai}) = k_x(x_{Ai} - x_{AL}) = N_A \qquad \text{Eq. 6.2.1.} - 12$$

The flux, N_A, can be written in terms of the overall mass transfer coefficients
The two expressions need to be the same because they represent the same flux

$$N_A = K_y(y_{AG} - y_A^*) = K_x(x_A^* - x_{AL}) \qquad \text{Eq. 6.2.1.} - 13$$

Recall that the equilibrium curve is a relationship between concentrations of a species in say, the liquid (x) and the gas (y) phases at equilibrium
If the equilibrium curve is linear, or can be considered to be piece-wise linear in the region of interest

$$y_{Ai} = m\,x_{Ai} \qquad \text{Eq. 6.2.1.} - 14$$

$$y_A^* = m\,x_{AL}$$

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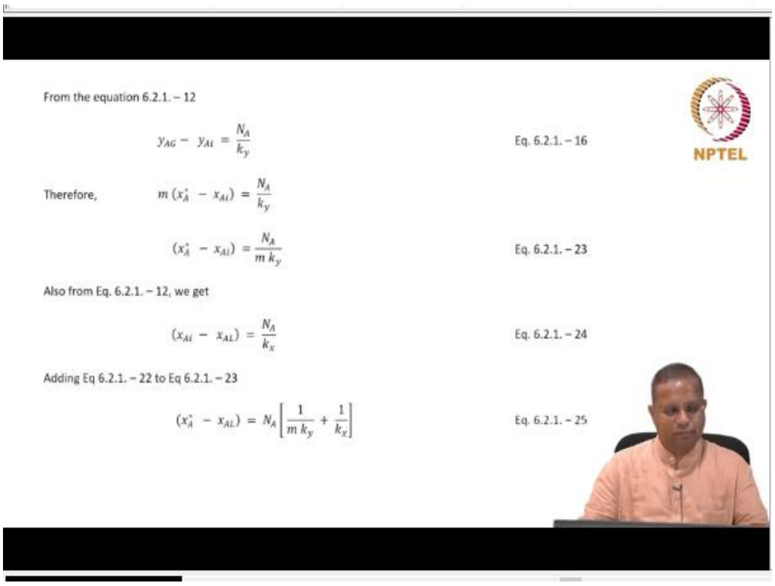

From the equation 6.2.1. – 12

$$y_{AG} - y_{Ai} = \frac{N_A}{k_y} \qquad \text{Eq. 6.2.1.} - 16$$

Therefore,
$$m\,(x_A^* - x_{Ai}) = \frac{N_A}{k_y}$$

$$(x_A^* - x_{Ai}) = \frac{N_A}{m\,k_y} \qquad \text{Eq. 6.2.1.} - 23$$

Also from Eq. 6.2.1. – 12, we get

$$(x_{Ai} - x_{AL}) = \frac{N_A}{k_x} \qquad \text{Eq. 6.2.1.} - 24$$

Adding Eq 6.2.1. – 22 to Eq 6.2.1. – 23

$$(x_A^* - x_{AL}) = N_A\left[\frac{1}{m\,k_y} + \frac{1}{k_x}\right] \qquad \text{Eq. 6.2.1.} - 25$$

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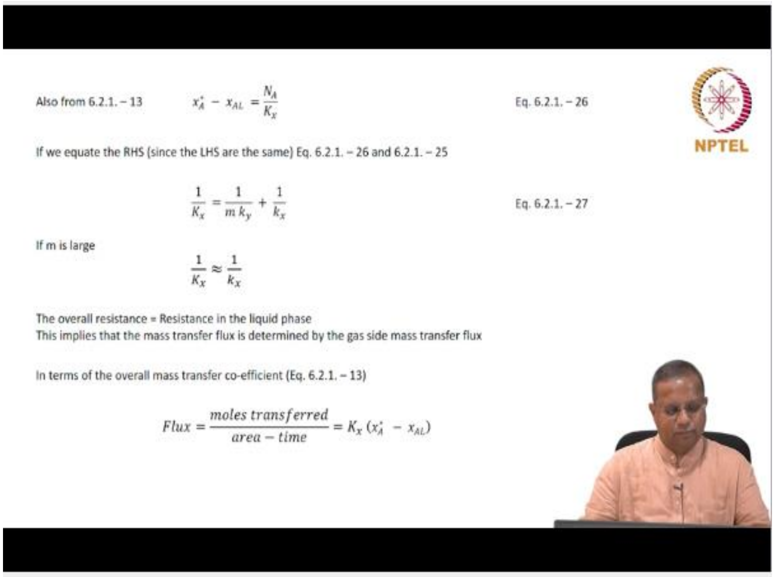

Also from 6.2.1. – 13 $x_A^* - x_{AL} = \frac{N_A}{K_x}$ Eq. 6.2.1. – 26

If we equate the RHS (since the LHS are the same) Eq. 6.2.1. – 26 and 6.2.1. – 25

$$\frac{1}{K_x} = \frac{1}{m\,k_y} + \frac{1}{k_x} \qquad \text{Eq. 6.2.1. – 27}$$

If m is large

$$\frac{1}{K_x} \approx \frac{1}{k_x}$$

The overall resistance = Resistance in the liquid phase
This implies that the mass transfer flux is determined by the gas side mass transfer flux

In terms of the overall mass transfer co-efficient (Eq. 6.2.1. – 13)

$$Flux = \frac{moles\ transferred}{area - time} = K_x\,(x_A^* - x_{AL})$$

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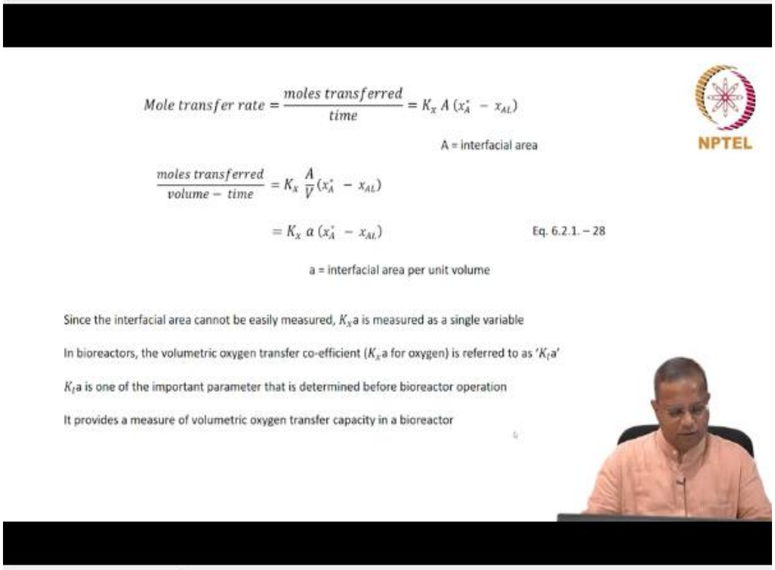

$$Mole\ transfer\ rate = \frac{moles\ transferred}{time} = K_x\,A\,(x_A^* - x_{AL})$$

A = interfacial area

$$\frac{moles\ transferred}{volume - time} = K_x\,\frac{A}{V}(x_A^* - x_{AL})$$

$$= K_x\,a\,(x_A^* - x_{AL}) \qquad \text{Eq. 6.2.1. – 28}$$

a = interfacial area per unit volume

Since the interfacial area cannot be easily measured, K_xa is measured as a single variable

In bioreactors, the volumetric oxygen transfer co-efficient (K_xa for oxygen) is referred to as 'K_la'

K_la is one of the important parameter that is determined before bioreactor operation

It provides a measure of volumetric oxygen transfer capacity in a bioreactor

So, what this gave us was a quantity called the k_La. K_x a which is referred to as a k_La which is the volumetric mass transfer coefficient, the volumetric it indicates the ability of a bioreactor to provide oxygen towards culture. And it is an important parameter we said pretty much its measured before every bioreactor run whether in the lab or in the industry.

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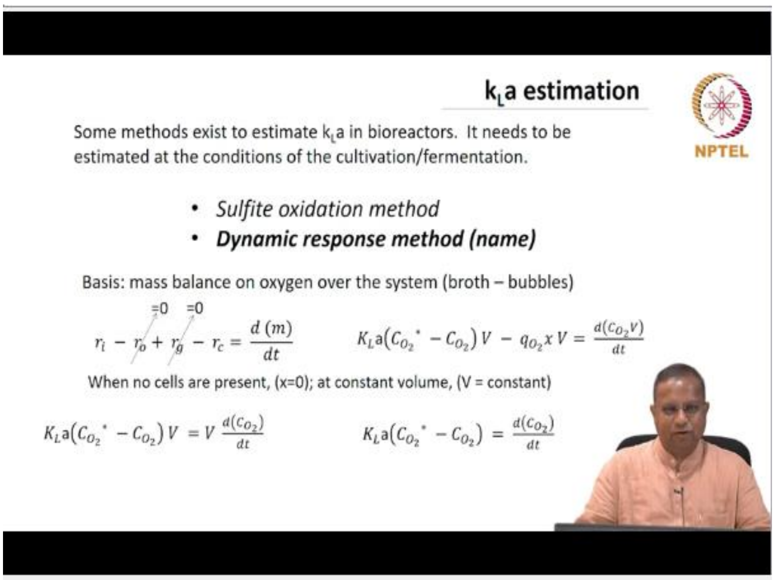

k_La estimation

Some methods exist to estimate k_La in bioreactors. It needs to be estimated at the conditions of the cultivation/fermentation.

- *Sulfite oxidation method*
- ***Dynamic response method (name)***

Basis: mass balance on oxygen over the system (broth – bubbles)

$$r_i - \overset{=0}{\cancel{r_o}} + \overset{=0}{\cancel{r_g}} - r_c = \frac{d\,(m)}{dt} \qquad K_L a\left(C_{O_2}{}^{*} - C_{O_2}\right)V - q_{O_2} x\,V = \frac{d(C_{O_2}V)}{dt}$$

When no cells are present, (x=0); at constant volume, (V = constant)

$$K_L a\left(C_{O_2}{}^{*} - C_{O_2}\right)V = V\,\frac{d(C_{O_2})}{dt} \qquad K_L a\left(C_{O_2}{}^{*} - C_{O_2}\right) = \frac{d(C_{O_2})}{dt}$$

And I also showed you how you could estimate k $_L$a by the dynamic response whether it came and discussed the dynamic response method in some detail. Sulphide oxidation is an old method we did not discuss it. Also I mentioned that we need to be careful with the name. The dynamic response method refers to different things in different textbooks. This is something that is common across many textbooks.

So I would use that and also we had used an intelligent system or you know, a very insightful system broth minus bubbles to get at simplifying the balance to get at a useful relationship to estimate k $_L$a from experimental data of oxygen sorption onto a liquid system.

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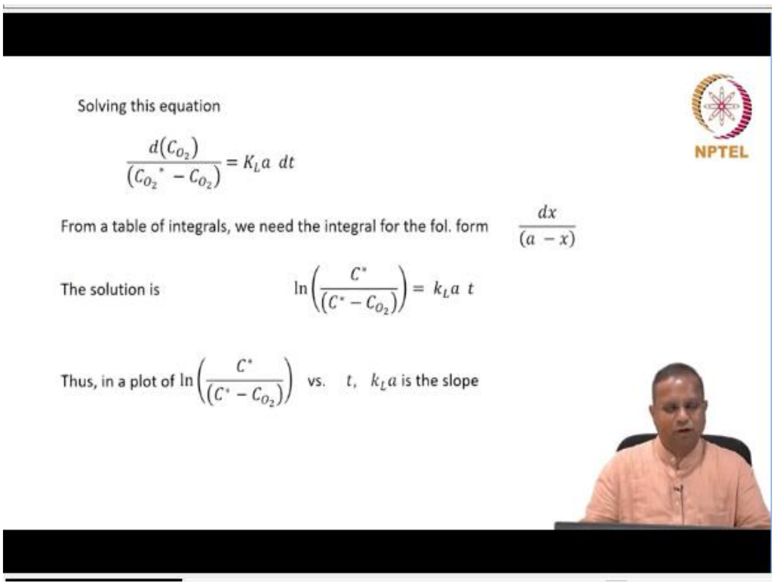

Solving this equation

$$\frac{d(C_{O_2})}{(C_{O_2}{}^{*} - C_{O_2})} = K_L a\ dt$$

From a table of integrals, we need the integral for the fol. form $\frac{dx}{(a\ - x)}$

The solution is $\ln\left(\frac{C^{*}}{(C^{*} - C_{O_2})}\right) = k_L a\ t$

Thus, in a plot of $\ln\left(\frac{C^{*}}{(C^{*} - C_{O_2})}\right)$ vs. t, $k_L a$ is the slope

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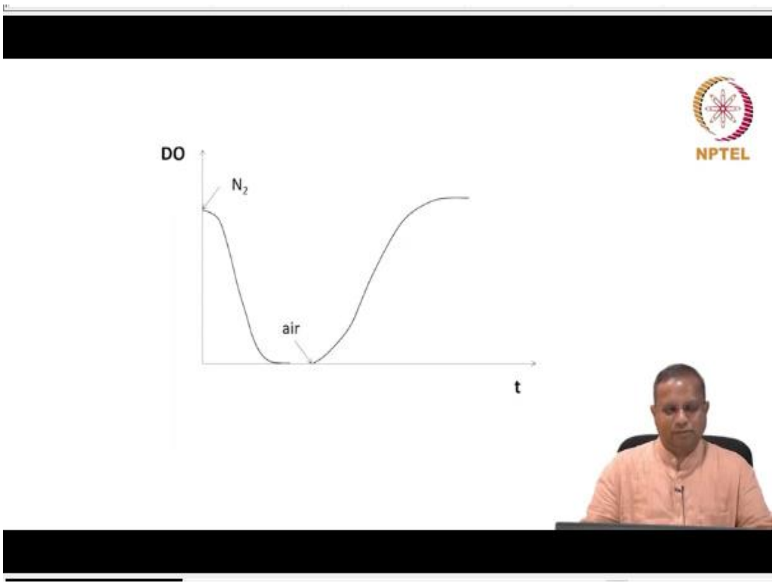

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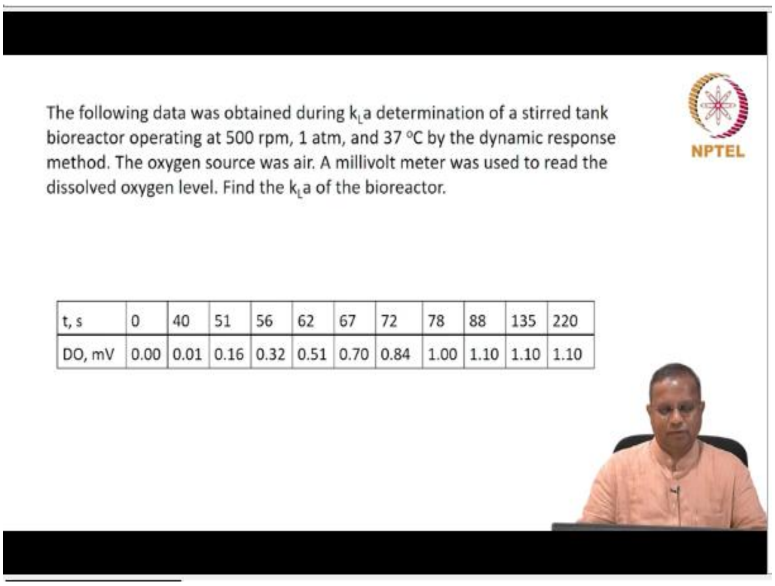

The following data was obtained during k_La determination of a stirred tank bioreactor operating at 500 rpm, 1 atm, and 37 °C by the dynamic response method. The oxygen source was air. A millivolt meter was used to read the dissolved oxygen level. Find the k_La of the bioreactor.

t, s	0	40	51	56	62	67	72	78	88	135	220
DO, mV	0.00	0.01	0.16	0.32	0.51	0.70	0.84	1.00	1.10	1.10	1.10

The bioreactor system that is we also worked at a problem to show how you could get to k_La from irrelevant data. This is from my PhD days, my own data okay.

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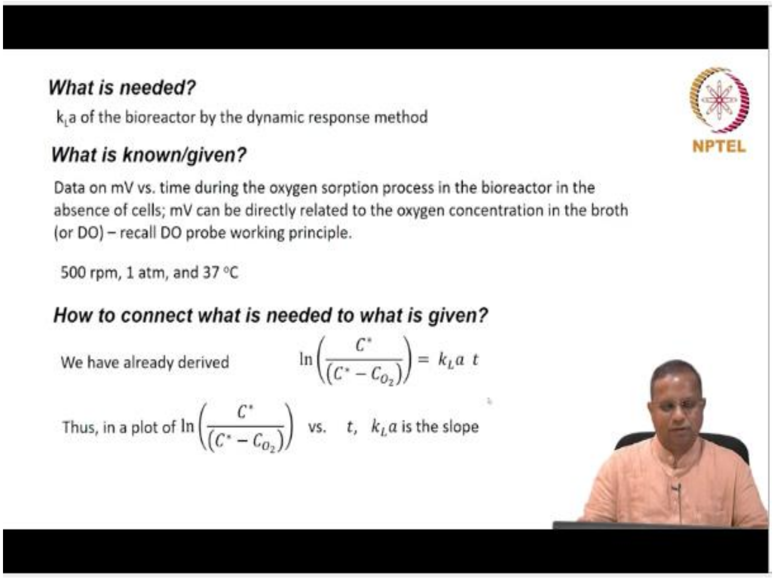

What is needed?

k_La of the bioreactor by the dynamic response method

What is known/given?

Data on mV vs. time during the oxygen sorption process in the bioreactor in the absence of cells; mV can be directly related to the oxygen concentration in the broth (or DO) – recall DO probe working principle.

500 rpm, 1 atm, and 37 °C

How to connect what is needed to what is given?

We have already derived $\ln\left(\frac{C^*}{(C^* - C_{O_2})}\right) = k_L a\ t$

Thus, in a plot of $\ln\left(\frac{C^*}{(C^* - C_{O_2})}\right)$ vs. t, $k_L a$ is the slope

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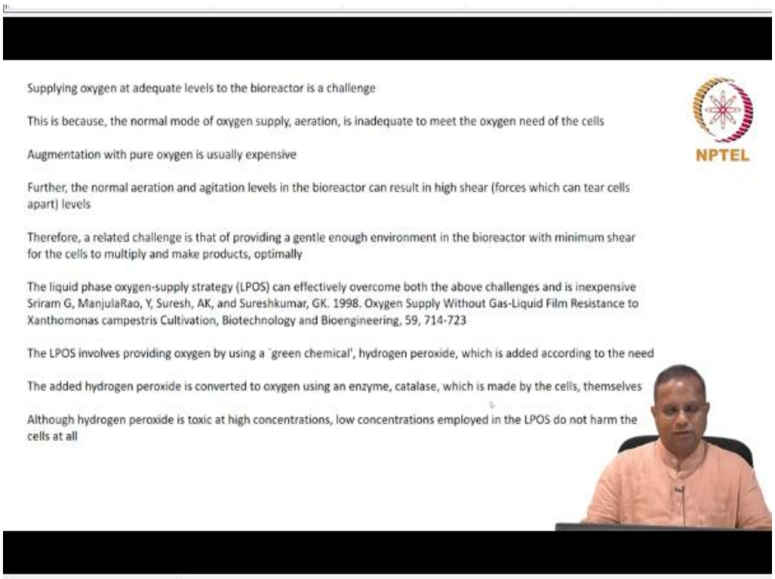

Supplying oxygen at adequate levels to the bioreactor is a challenge

This is because, the normal mode of oxygen supply, aeration, is inadequate to meet the oxygen need of the cells

Augmentation with pure oxygen is usually expensive

Further, the normal aeration and agitation levels in the bioreactor can result in high shear (forces which can tear cells apart) levels

Therefore, a related challenge is that of providing a gentle enough environment in the bioreactor with minimum shear for the cells to multiply and make products, optimally

The liquid phase oxygen-supply strategy (LPOS) can effectively overcome both the above challenges and is inexpensive
Sriram G, ManjulaRao, Y, Suresh, AK, and Sureshkumar, GK. 1998. Oxygen Supply Without Gas-Liquid Film Resistance to Xanthomonas campestris Cultivation, Biotechnology and Bioengineering, 59, 714-723

The LPOS involves providing oxygen by using a `green chemical', hydrogen peroxide, which is added according to the need

The added hydrogen peroxide is converted to oxygen using an enzyme, catalase, which is made by the cells, themselves

Although hydrogen peroxide is toxic at high concentrations, low concentrations employed in the LPOS do not harm the cells at all

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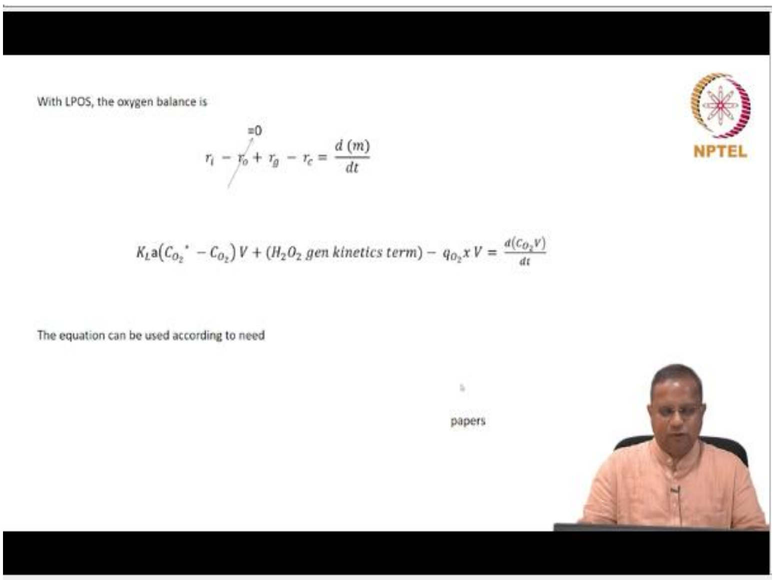

With LPOS, the oxygen balance is

$$r_i - \overset{=0}{\cancel{r_o}} + r_g - r_c = \frac{d\,(m)}{dt}$$

$$K_L a\left(C_{O_2}{}^{*} - C_{O_2}\right)V + (H_2O_2\ gen\ kinetics\ term) - q_{O_2}x\,V = \frac{d(C_{O_2}V)}{dt}$$

The equation can be used according to need

papers

That was for the problem, okay. Then we will talk a little bit about the quite a lot about the liquid phase oxygen supply strategy, where you have a generation term also coming in through hydrogen peroxide and so on so forth. And then I went off into the research significance of transport principles. They are principles that can be applied anywhere. I gave you a flavor of how they were applied to get to some very meaningful aspects in our own research.

And I think I discussed about 4 or 5 papers starting with the LPOS paper and all the way down, including the most one of the recent papers on which had used the principle of pseudo steady state, pseudo steady state approximation to get at very meaningful insights, which can also have the ability to transform the way medicine is done and so on and so forth. Okay, that's what we talked about okay.

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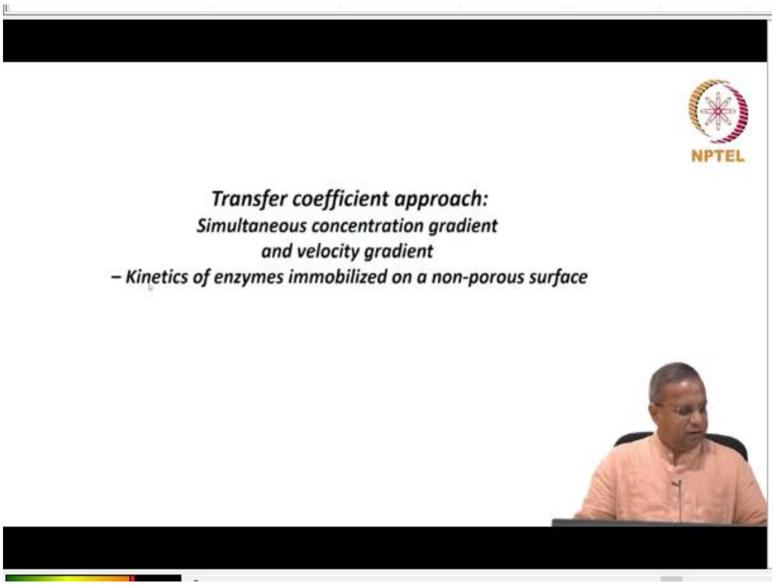

Transfer coefficient approach:
Simultaneous concentration gradient
and velocity gradient
– Kinetics of enzymes immobilized on a non-porous surface

You can go and refer to those papers, get more out of it. If you have any comments or questions, please raise them in the asked a question forum. Then we went back and looked at the concentration and velocity gradients, velocity and temperature gradients from an equations point of view. We have some time so I can probably tell you that okay. First was the application to the enzyme immobilized on a non porous surface the process kinetics of that okay.

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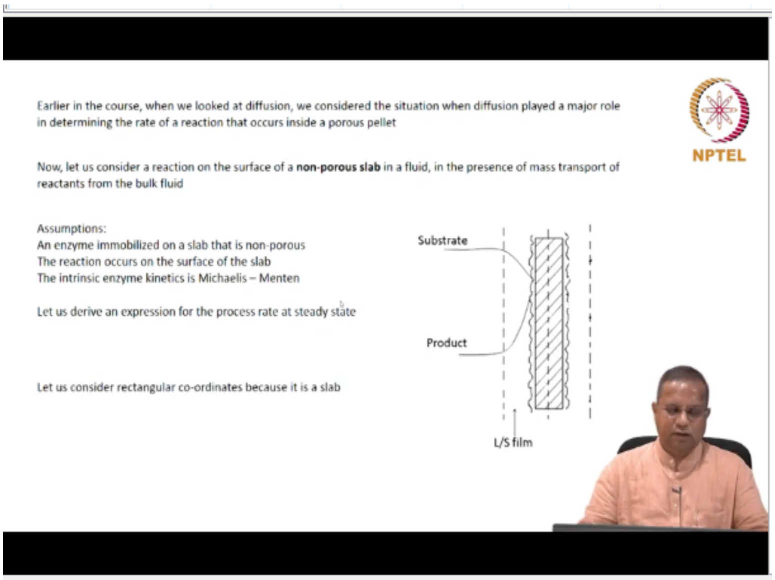

Earlier in the course, when we looked at diffusion, we considered the situation when diffusion played a major role in determining the rate of a reaction that occurs inside a porous pellet

Now, let us consider a reaction on the surface of a **non-porous slab** in a fluid, in the presence of mass transport of reactants from the bulk fluid

Assumptions:
An enzyme immobilized on a slab that is non-porous
The reaction occurs on the surface of the slab
The intrinsic enzyme kinetics is Michaelis – Menten

Let us derive an expression for the process rate at steady state

Let us consider rectangular co-ordinates because it is a slab

We said that let me go to this picture, up to we said that this is a slab, a cuboidal that sits in the liquid, so it is a rectangle in section. So, you have an enzyme that is immobilized onto the surface of the slab, you have a substrate that goes from the bulk to this enzyme crushing the liquid solid film and then the product that moves out okay. There is an aspect of transport associated with substrates moving from the bulk to the interface.

And then the product moving out and then there is an aspect of the reaction itself. These 2 have certain characteristic times associated with it and the process time depends on the characteristic times of transport and reaction. So, which one is important, it can be inferred from what is called an effectiveness factor. The Damkohler number gives you some idea in terms of a general view and so on and so forth.

And to model S gives you some idea in terms of extremes, the view of extremes in that particular situation, whereas, effectiveness factor gives you which one is more important.

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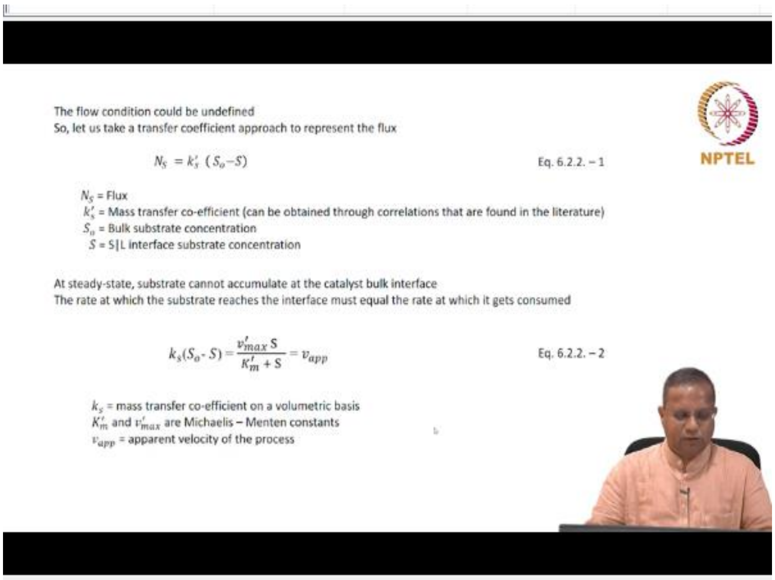

The flow condition could be undefined
So, let us take a transfer coefficient approach to represent the flux

$$N_S = k_s' \ (S_o - S) \qquad \text{Eq. 6.2.2.} - 1$$

N_S = Flux
k_s' = Mass transfer co-efficient (can be obtained through correlations that are found in the literature)
S_o = Bulk substrate concentration
S = S|L interface substrate concentration

At steady-state, substrate cannot accumulate at the catalyst bulk interface
The rate at which the substrate reaches the interface must equal the rate at which it gets consumed

$$k_s(S_o - S) = \frac{v'_{max}\,\mathrm{S}}{K'_m + \mathrm{S}} = v_{app} \qquad \text{Eq. 6.2.2.} - 2$$

k_s = mass transfer co-efficient on a volumetric basis
K'_m and v'_{max} are Michaelis – Menten constants
v_{app} = apparent velocity of the process

To get to such insights, we had used the transcription approach for one compared it with the reaction rate.

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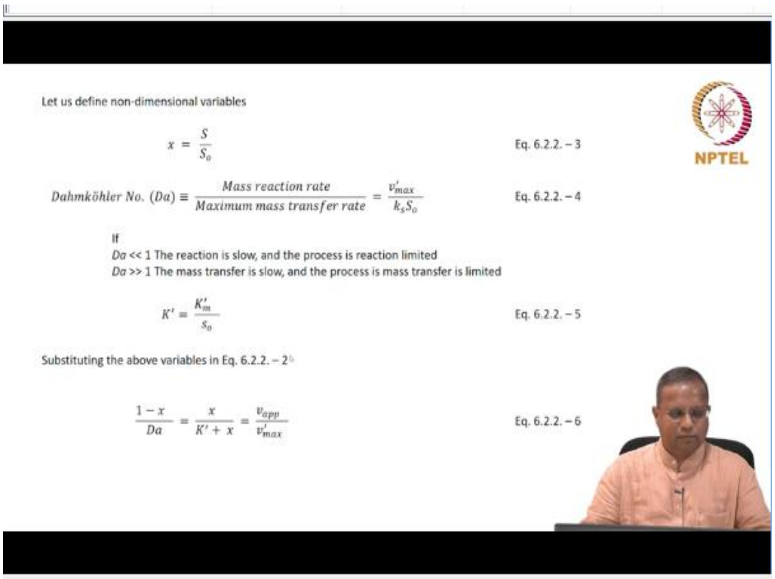

Let us define non-dimensional variables

$$x = \frac{S}{S_o} \qquad \text{Eq. 6.2.2.} - 3$$

$$\text{Dahmk\"ohler No. } (Da) \equiv \frac{\text{Mass reaction rate}}{\text{Maximum mass transfer rate}} = \frac{v'_{max}}{k_s S_o} \qquad \text{Eq. 6.2.2.} - 4$$

If
$Da \ll 1$ The reaction is slow, and the process is reaction limited
$Da \gg 1$ The mass transfer is slow, and the process is mass transfer is limited

$$K' = \frac{K'_m}{S_o} \qquad \text{Eq. 6.2.2.} - 5$$

Substituting the above variables in Eq. 6.2.2. – 2

$$\frac{1-x}{Da} = \frac{x}{K' + x} = \frac{v_{app}}{v'_{max}} \qquad \text{Eq. 6.2.2.} - 6$$

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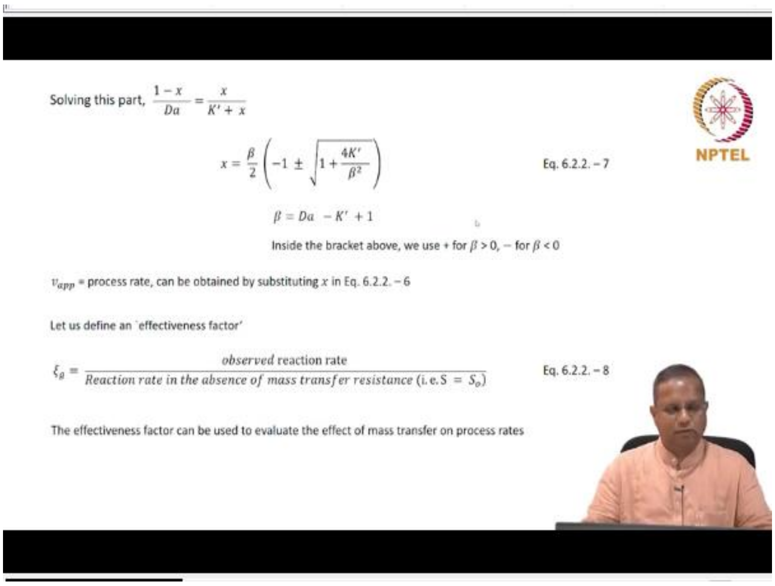

Solving this part, $\frac{1-x}{Da} = \frac{x}{K'+x}$

$$x = \frac{\beta}{2}\left(-1 \pm \sqrt{1+\frac{4K'}{\beta^2}}\right) \qquad \text{Eq. 6.2.2.} - 7$$

$$\beta = Da \;- K' + 1$$

Inside the bracket above, we use + for $\beta > 0$, − for $\beta < 0$

v_{app} = process rate, can be obtained by substituting x in Eq. 6.2.2. − 6

Let us define an 'effectiveness factor'

$$\xi_g = \frac{observed \text{ reaction rate}}{Reaction\ rate\ in\ the\ absence\ of\ mass\ transfer\ resistance\ (\text{i.e.} S = S_o)} \qquad \text{Eq. 6.2.2.} - 8$$

The effectiveness factor can be used to evaluate the effect of mass transfer on process rates

And we had gone through the derivation, effectiveness factor is the ratio of the observed reaction rate to the reaction rate in the absence of mass transfer resistance. And this is what gives you all the insights at that I just spoke about it.

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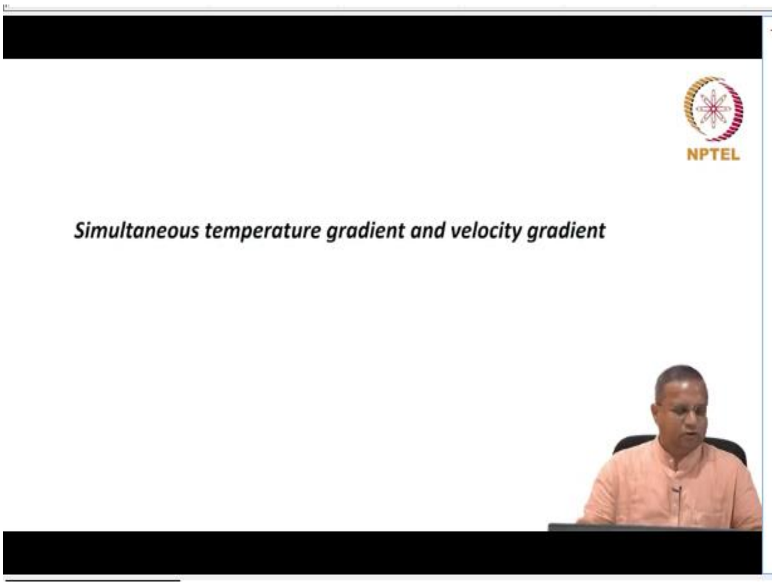

Simultaneous temperature gradient and velocity gradient

Then we continued with the equations approach for simultaneous temperature gradient and velocity gradient. In this case it was heating of a protein solution in a horizontal cylindrical tube.

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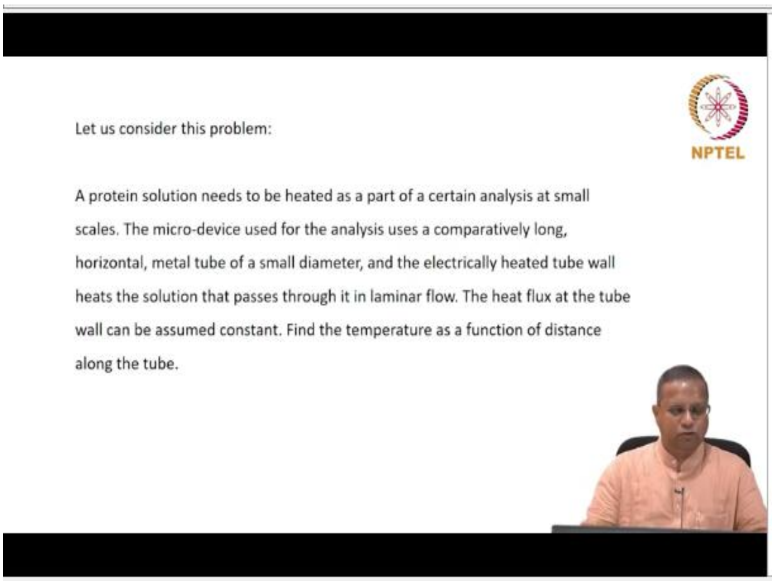

Let us consider this problem:

A protein solution needs to be heated as a part of a certain analysis at small scales. The micro-device used for the analysis uses a comparatively long, horizontal, metal tube of a small diameter, and the electrically heated tube wall heats the solution that passes through it in laminar flow. The heat flux at the tube wall can be assumed constant. Find the temperature as a function of distance along the tube.

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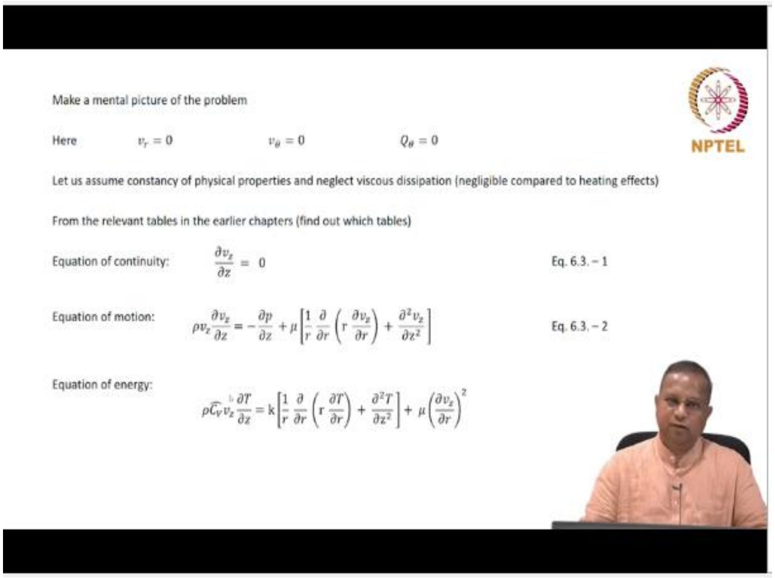

Make a mental picture of the problem

Here $v_r = 0$ $v_\theta = 0$ $Q_\theta = 0$

Let us assume constancy of physical properties and neglect viscous dissipation (negligible compared to heating effects)

From the relevant tables in the earlier chapters (find out which tables)

Equation of continuity: $$\frac{\partial v_z}{\partial z} = 0$$ Eq. 6.3. – 1

Equation of motion: $$\rho v_z \frac{\partial v_z}{\partial z} = -\frac{\partial p}{\partial z} + \mu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right) + \frac{\partial^2 v_z}{\partial z^2}\right]$$ Eq. 6.3. – 2

Equation of energy:

$$\rho \widehat{C}_V v_z \frac{\partial T}{\partial z} = k\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right] + \mu\left(\frac{\partial v_z}{\partial r}\right)^2$$

We said we needed to solve the equation of continuity, equation of motion and the equation of energy simultaneously.

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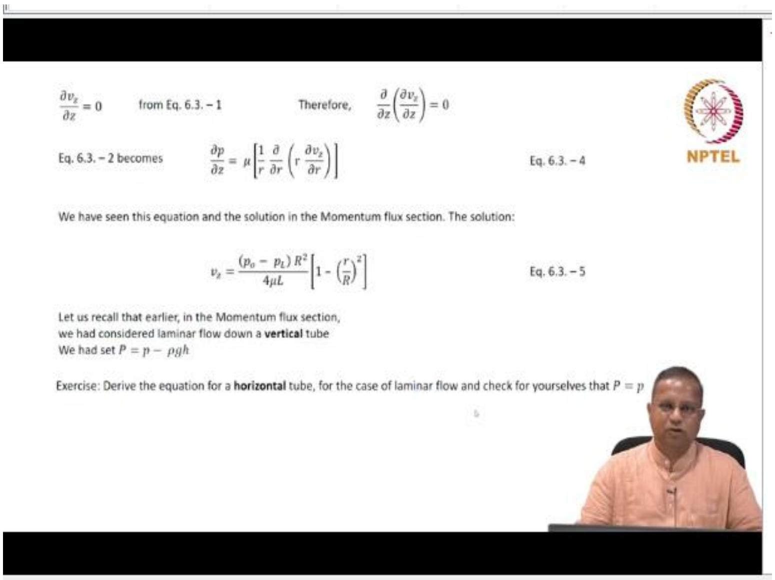

$\frac{\partial v_z}{\partial z} = 0$ from Eq. 6.3. – 1 Therefore, $\frac{\partial}{\partial z}\left(\frac{\partial v_z}{\partial z}\right) = 0$

Eq. 6.3. – 2 becomes $\frac{\partial p}{\partial z} = \mu\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial v_z}{\partial r}\right)\right]$ Eq. 6.3. – 4

We have seen this equation and the solution in the Momentum flux section. The solution:

$$v_z = \frac{(p_o - p_L)R^2}{4\mu L}\left[1 - \left(\frac{r}{R}\right)^2\right] \qquad \text{Eq. 6.3. – 5}$$

Let us recall that earlier, in the Momentum flux section,
we had considered laminar flow down a **vertical** tube
We had set $P = p - \rho g h$

Exercise: Derive the equation for a **horizontal** tube, for the case of laminar flow and check for yourselves that $P = p$

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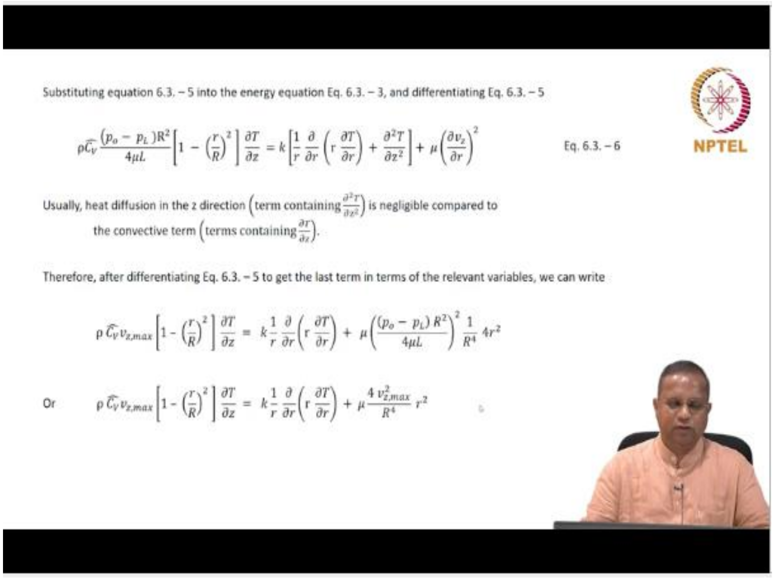

Substituting equation 6.3. – 5 into the energy equation Eq. 6.3. – 3, and differentiating Eq. 6.3. – 5

$$\rho\widehat{C_V}\frac{(p_o - p_L)R^2}{4\mu L}\left[1 - \left(\frac{r}{R}\right)^2\right]\frac{\partial T}{\partial z} = k\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right] + \mu\left(\frac{\partial v_z}{\partial r}\right)^2 \qquad \text{Eq. 6.3. – 6}$$

Usually, heat diffusion in the z direction $\left(\text{term containing}\frac{\partial^2 T}{\partial z^2}\right)$ is negligible compared to the convective term $\left(\text{terms containing}\frac{\partial T}{\partial z}\right)$.

Therefore, after differentiating Eq. 6.3. – 5 to get the last term in terms of the relevant variables, we can write

$$\rho\,\widehat{C_V}v_{z,max}\left[1 - \left(\frac{r}{R}\right)^2\right]\frac{\partial T}{\partial z} = k\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \mu\left(\frac{(p_o - p_L)R^2}{4\mu L}\right)^2\frac{1}{R^4}4r^2$$

Or $$\rho\,\widehat{C_V}v_{z,max}\left[1 - \left(\frac{r}{R}\right)^2\right]\frac{\partial T}{\partial z} = k\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \mu\frac{4\,v_{z,max}^2}{R^4}r^2$$

Then we did that and got an analytical solution at least for the limiting case.

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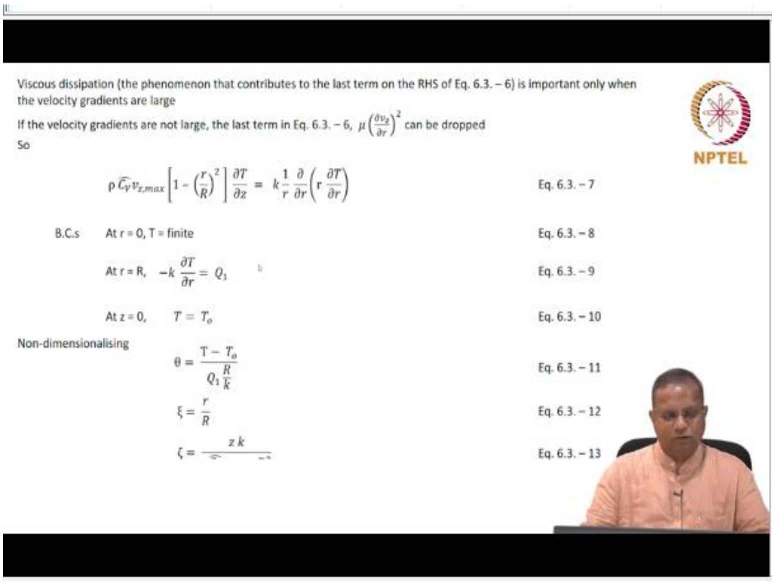

Viscous dissipation (the phenomenon that contributes to the last term on the RHS of Eq. 6.3. – 6) is important only when the velocity gradients are large

If the velocity gradients are not large, the last term in Eq. 6.3. – 6, $\mu\left(\frac{\partial v_z}{\partial r}\right)^2$ can be dropped

So

$$\rho\,\widehat{C}_V v_{z,max}\left[1-\left(\frac{r}{R}\right)^2\right]\frac{\partial T}{\partial z} = k\frac{1}{r}\frac{\partial}{\partial r}\left(r\,\frac{\partial T}{\partial r}\right) \qquad \text{Eq. 6.3.} - 7$$

B.C.s At r = 0, T = finite Eq. 6.3. – 8

At r = R, $-k\,\frac{\partial T}{\partial r} = Q_1$ Eq. 6.3. – 9

At z = 0, $T = T_o$ Eq. 6.3. – 10

Non-dimensionalising

$$\theta = \frac{T - T_o}{Q_1\frac{R}{k}} \qquad \text{Eq. 6.3.} - 11$$

$$\xi = \frac{r}{R} \qquad \text{Eq. 6.3.} - 12$$

$$\zeta = \frac{z\,k}{} \qquad \text{Eq. 6.3.} - 13$$

I also mentioned that you could get, you could also use numerical methods to solve them if you have the skill or if you can team up with the person with the right skills in numerical solutions, numerical analysis, numerical solutions and so on so forth.

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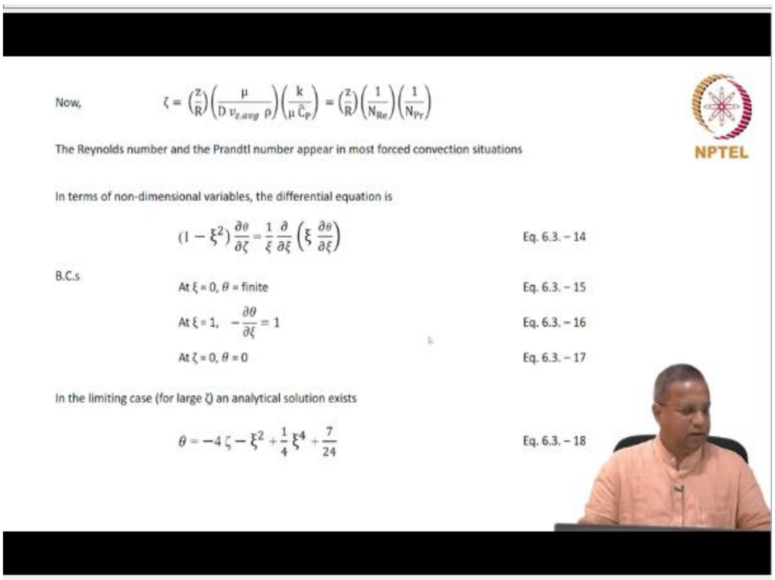

Now, $\zeta = \left(\frac{z}{R}\right)\left(\frac{\mu}{D\,v_{z,avg}\,\rho}\right)\left(\frac{k}{\mu\,\hat{C}_P}\right) = \left(\frac{z}{R}\right)\left(\frac{1}{N_{Re}}\right)\left(\frac{1}{N_{Pr}}\right)$

The Reynolds number and the Prandtl number appear in most forced convection situations

In terms of non-dimensional variables, the differential equation is

$$(1-\xi^2)\,\frac{\partial\theta}{\partial\zeta} = \frac{1}{\xi}\,\frac{\partial}{\partial\xi}\left(\xi\,\frac{\partial\theta}{\partial\xi}\right) \qquad \text{Eq. 6.3.} - 14$$

B.C.s

At $\xi = 0$, θ = finite Eq. 6.3. – 15

At $\xi = 1$, $-\frac{\partial\theta}{\partial\xi} = 1$ Eq. 6.3. – 16

At $\zeta = 0$, $\theta = 0$ Eq. 6.3. – 17

In the limiting case (for large ζ) an analytical solution exists

$$\theta = -4\,\zeta - \xi^2 + \frac{1}{4}\,\xi^4 + \frac{7}{24} \qquad \text{Eq. 6.3.} - 18$$

Okay then we saw the occurrence of the Reynolds number and Prandtl number in most of these forced convection situations, these are non dimensional numbers which have great significance, we already know the significance of the non dimensional numbers okay.

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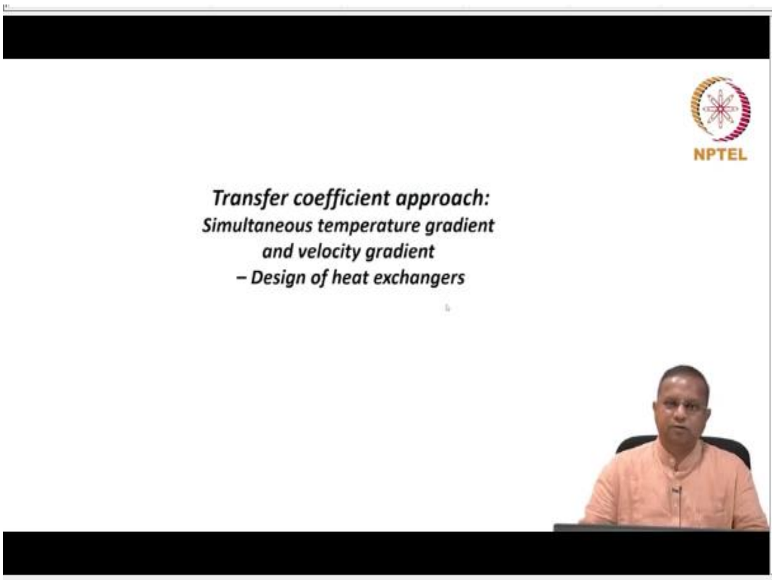

Transfer coefficient approach:
Simultaneous temperature gradient
and velocity gradient
– Design of heat exchangers

And I think after that, we got into the last part which was using or taking the transfer coefficient approach, we use a heat transfer coefficient for design of heat exchangers, heat exchangers are important equipment in the industry. And there are principles that govern it although they are the size of entire rooms and so on so forth. There are principles that govern these.

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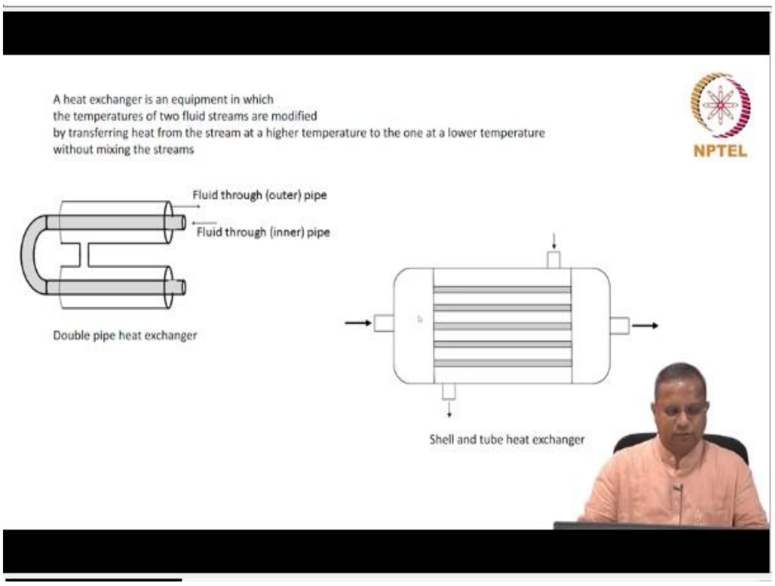

A heat exchanger is an equipment in which
the temperatures of two fluid streams are modified
by transferring heat from the stream at a higher temperature to the one at a lower temperature
without mixing the streams

And some of the principles we saw in this course. We took an example of changing the temperature of an algal broth that had heated up by passing through the photo section, right.

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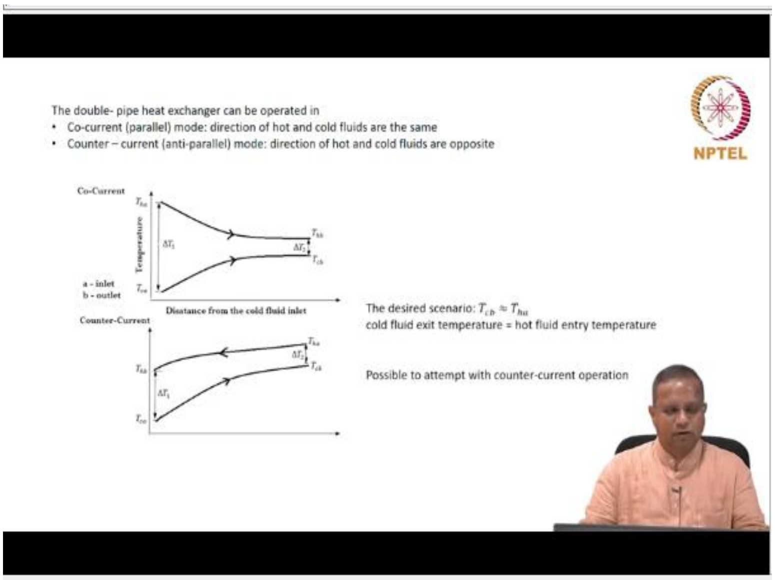

The double- pipe heat exchanger can be operated in

- Co-current (parallel) mode: direction of hot and cold fluids are the same
- Counter – current (anti-parallel) mode: direction of hot and cold fluids are opposite

The desired scenario: $T_{cb} \approx T_{ha}$
cold fluid exit temperature = hot fluid entry temperature

Possible to attempt with counter-current operation

Okay, that is the example that we took to provide us with the context in which to pick up these principles. So, we had as a result looked co-current flow, counter current flow.

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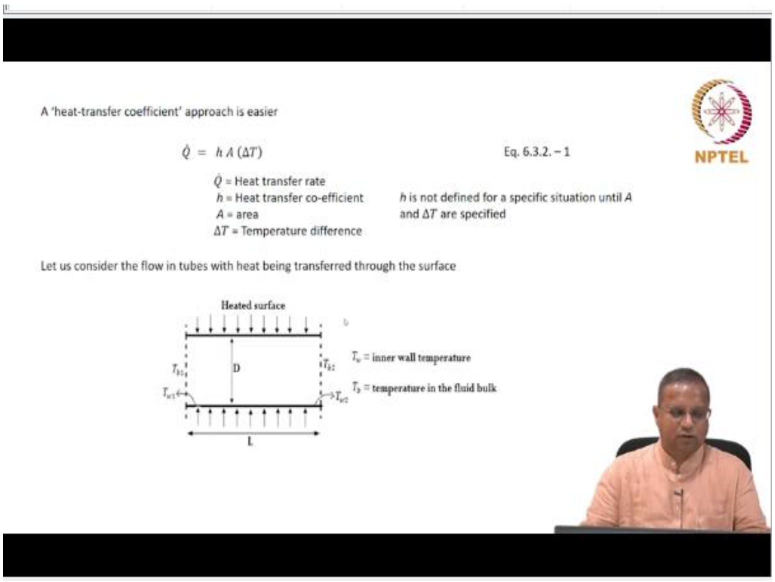

A 'heat-transfer coefficient' approach is easier

$$\dot{Q} = h A (\Delta T) \qquad \text{Eq. 6.3.2. – 1}$$

$\dot{Q}$ = Heat transfer rate
h = Heat transfer co-efficient
A = area
ΔT = Temperature difference

h is not defined for a specific situation until A and ΔT are specified

Let us consider the flow in tubes with heat being transferred through the surface

T_w = inner wall temperature
T_b = temperature in the fluid bulk

Then this simple equation as was the basis, h A ΔT is the heat transfer rate, we saw different kinds of heat transfer coefficients, and that it depends on the kind of temperature difference that we talking about and the kind of areas that we're talking about.

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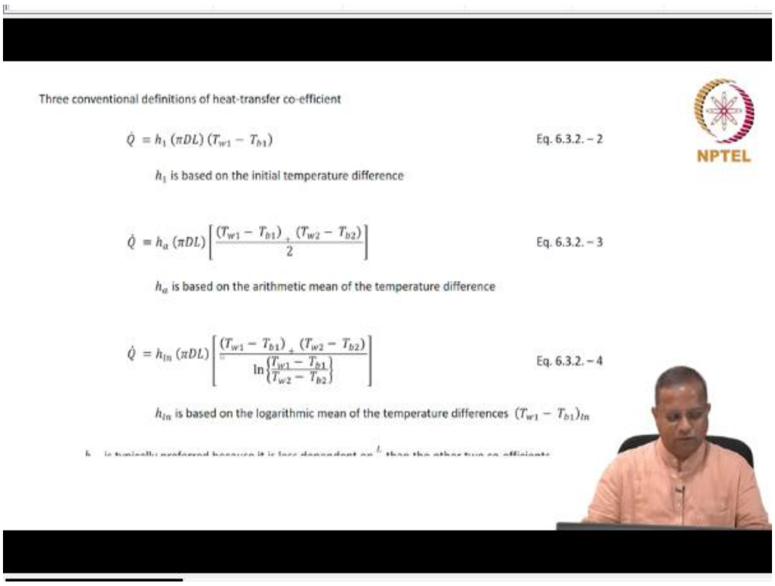

Three conventional definitions of heat-transfer co-efficient

$$\dot{Q} = h_1 (\pi DL)(T_{w1} - T_{b1}) \qquad \text{Eq. 6.3.2.} - 2$$

h_1 is based on the initial temperature difference

$$\dot{Q} = h_a (\pi DL)\left[\frac{(T_{w1} - T_{b1}) + (T_{w2} - T_{b2})}{2}\right] \qquad \text{Eq. 6.3.2.} - 3$$

h_a is based on the arithmetic mean of the temperature difference

$$\dot{Q} = h_{ln} (\pi DL)\left[\frac{(T_{w1} - T_{b1}) + (T_{w2} - T_{b2})}{\ln\left\{\frac{T_{w1} - T_{b1}}{T_{w2} - T_{b2}}\right\}}\right] \qquad \text{Eq. 6.3.2.} - 4$$

h_{ln} is based on the logarithmic mean of the temperature differences $(T_{w1} - T_{b1})_{ln}$

There are 3 different types the heat transfer function based on the initial temperature difference, then the heat transfer coefficient on based on the arithmetic mean of the temperature differences. And then the heat transfer coefficient based on the logarithmic mean of the temperature differences, this is preferred because it depends less on πLD and so on and so forth.

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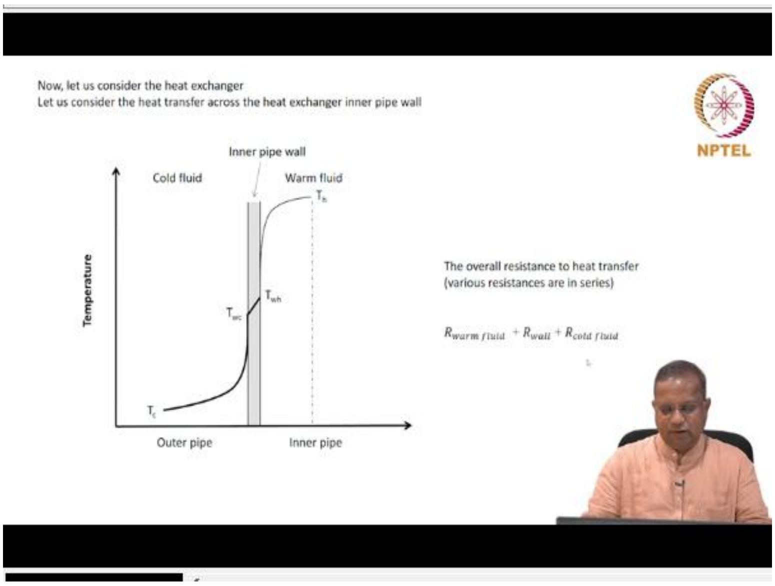

Now, let us consider the heat exchanger
Let us consider the heat transfer across the heat exchanger inner pipe wall

The overall resistance to heat transfer
(various resistances are in series)

$$R_{warm\ fluid} + R_{wall} + R_{cold\ fluid}$$

Okay. Then a differential approach was introduced then the basis for heat exchanger design was presented. This was the starting point, the total resistance of the various resistances and series were considered.

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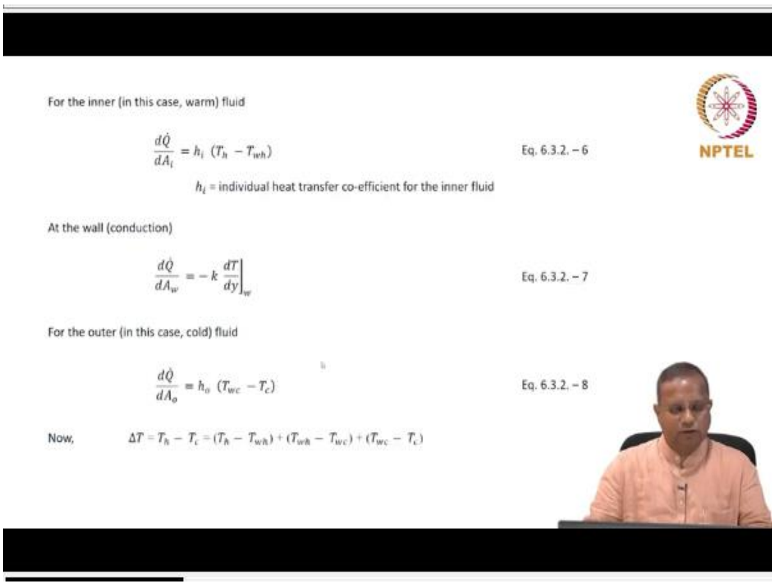

For the inner (in this case, warm) fluid

$$\frac{d\dot{Q}}{dA_i} = h_i\ (T_h - T_{wh}) \qquad \text{Eq. 6.3.2.} - 6$$

h_i = individual heat transfer co-efficient for the inner fluid

At the wall (conduction)

$$\frac{d\dot{Q}}{dA_w} = -k\ \frac{dT}{dy}\bigg|_w \qquad \text{Eq. 6.3.2.} - 7$$

For the outer (in this case, cold) fluid

$$\frac{d\dot{Q}}{dA_o} = h_o\ (T_{wc} - T_c) \qquad \text{Eq. 6.3.2.} - 8$$

Now, $\Delta T = T_h - T_c = (T_h - T_{wh}) + (T_{wh} - T_{wc}) + (T_{wc} - T_c)$

And then we wrote down expressions in terms of the heat transfer coefficient.

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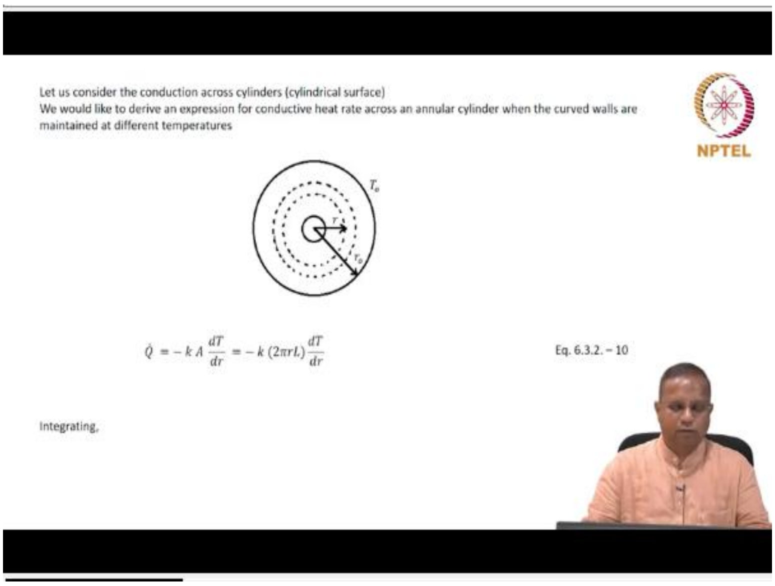

Let us consider the conduction across cylinders (cylindrical surface)
We would like to derive an expression for conductive heat rate across an annular cylinder when the curved walls are maintained at different temperatures

$$\dot{Q} = -k\,A\,\frac{dT}{dr} = -k\,(2\pi rL)\,\frac{dT}{dr} \qquad \text{Eq. 6.3.2.} - 10$$

Integrating,

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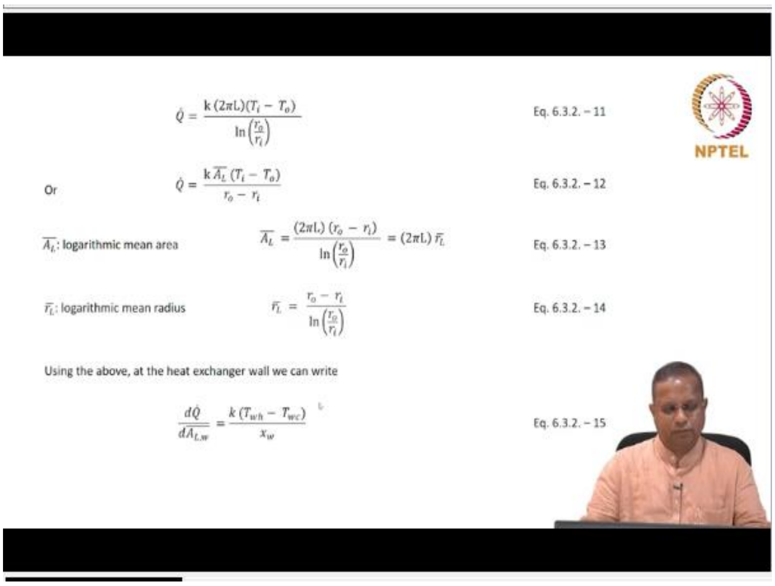

$$\dot{Q} = \frac{k\,(2\pi L)(T_i - T_o)}{\ln\left(\frac{r_o}{r_i}\right)}$$ Eq. 6.3.2. – 11

Or $$\dot{Q} = \frac{k\,\overline{A_L}\,(T_i - T_o)}{r_o - r_i}$$ Eq. 6.3.2. – 12

$\overline{A_L}$: logarithmic mean area $$\overline{A_L} = \frac{(2\pi L)\,(r_o - r_i)}{\ln\left(\frac{r_o}{r_i}\right)} = (2\pi L)\,\overline{r_L}$$ Eq. 6.3.2. – 13

$\overline{r_L}$: logarithmic mean radius $$\overline{r_L} = \frac{r_o - r_i}{\ln\left(\frac{r_o}{r_i}\right)}$$ Eq. 6.3.2. – 14

Using the above, at the heat exchanger wall we can write

$$\frac{d\dot{Q}}{d\overline{A}_{L,w}} = \frac{k\,(T_{wh} - T_{wc})}{x_w}$$ Eq. 6.3.2. – 15

To back out and overall heat transfer coefficient and there are 2 types based on the outer area of the inner pipe or the inner area of the inner pipe.

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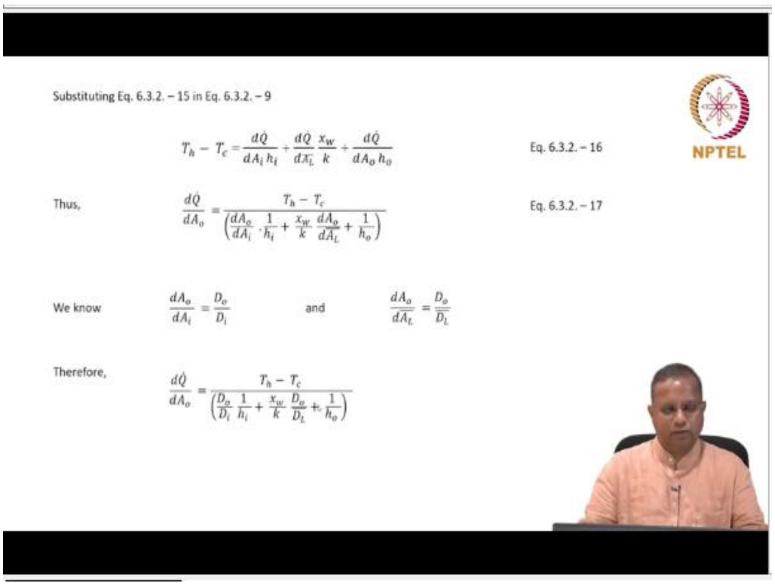

Substituting Eq. 6.3.2. – 15 in Eq. 6.3.2. – 9

$$T_h - T_c = \frac{d\dot{Q}}{dA_i\,h_i} + \frac{d\dot{Q}}{d\overline{A_L}}\frac{x_w}{k} + \frac{d\dot{Q}}{dA_o\,h_o}$$ Eq. 6.3.2. – 16

Thus, $$\frac{d\dot{Q}}{dA_o} = \frac{T_h - T_c}{\left(\frac{dA_o}{dA_i}\cdot\frac{1}{h_i} + \frac{x_w}{k}\frac{dA_o}{d\overline{A_L}} + \frac{1}{h_o}\right)}$$ Eq. 6.3.2. – 17

We know $\frac{dA_o}{dA_i} = \frac{D_o}{D_i}$ and $\frac{dA_o}{d\overline{A_L}} = \frac{D_o}{\overline{D_L}}$

Therefore, $$\frac{d\dot{Q}}{dA_o} = \frac{T_h - T_c}{\left(\frac{D_o}{D_i}\frac{1}{h_i} + \frac{x_w}{k}\frac{D_o}{\overline{D_L}} + \frac{1}{h_o}\right)}$$

All that we saw.

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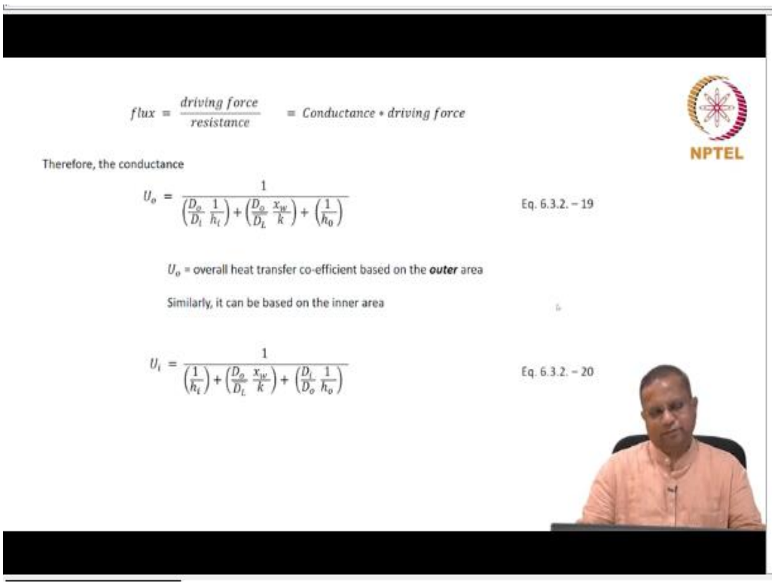

$$flux = \frac{driving\ force}{resistance} \quad = Conductance * driving\ force$$

Therefore, the conductance

$$U_o = \frac{1}{\left(\frac{D_o}{D_i}\frac{1}{h_i}\right) + \left(\frac{D_o}{D_L}\frac{x_w}{k}\right) + \left(\frac{1}{h_0}\right)} \qquad \text{Eq. 6.3.2.} - 19$$

U_o = overall heat transfer co-efficient based on the ***outer*** area

Similarly, it can be based on the inner area

$$U_i = \frac{1}{\left(\frac{1}{h_i}\right) + \left(\frac{D_o}{D_L}\frac{x_w}{k}\right) + \left(\frac{D_i}{D_o}\frac{1}{h_o}\right)} \qquad \text{Eq. 6.3.2.} - 20$$

And then, once you know that it is nothing but you can get the heat transfer rates just by $U_0 A \Delta T$. That is it.

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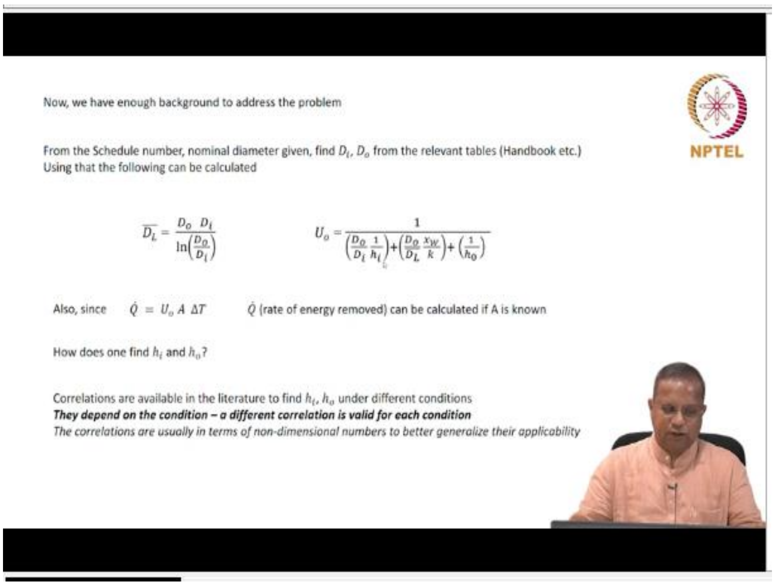

Now, we have enough background to address the problem

From the Schedule number, nominal diameter given, find D_i, D_o from the relevant tables (Handbook etc.)
Using that the following can be calculated

$$\overline{D_L} = \frac{D_o\ D_i}{\ln\left(\frac{D_o}{D_i}\right)} \qquad U_o = \frac{1}{\left(\frac{D_o}{D_i}\frac{1}{h_i}\right) + \left(\frac{D_o}{D_L}\frac{x_w}{k}\right) + \left(\frac{1}{h_0}\right)}$$

Also, since $\dot{Q} = U_o\ A\ \Delta T$ $\dot{Q}$ (rate of energy removed) can be calculated if A is known

How does one find h_i and h_o?

Correlations are available in the literature to find h_i, h_o under different conditions
They depend on the condition – a different correlation is valid for each condition
The correlations are usually in terms of non-dimensional numbers to better generalize their applicability

As simple as that. So, we came down to the fact that once you know the individual heat transfer coefficients, then you can get the overall heat transfer coefficient. The individual heat transfer coefficient you have a different correlation for different conditions.

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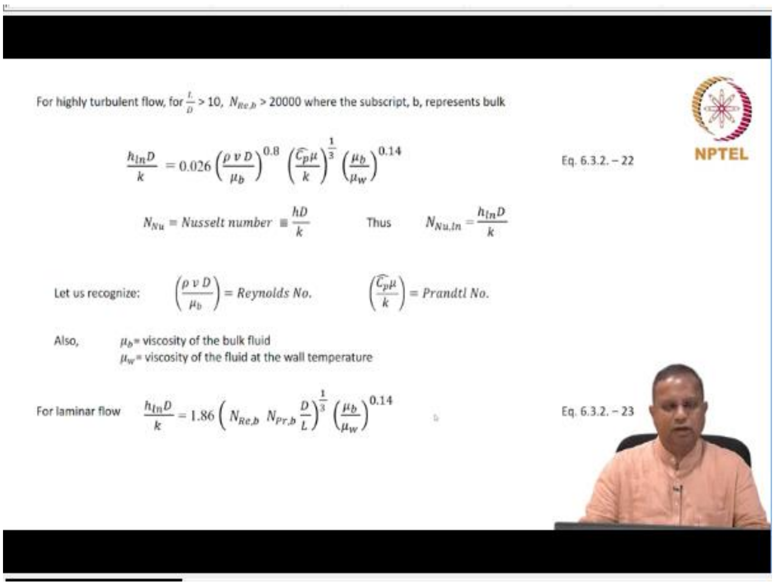

For highly turbulent flow, for $\frac{L}{D} > 10$, $N_{Re,b} > 20000$ where the subscript, b, represents bulk

$$\frac{h_{ln}D}{k} = 0.026\left(\frac{\rho\, v\, D}{\mu_b}\right)^{0.8}\left(\frac{\widehat{C_p}\mu}{k}\right)^{\frac{1}{3}}\left(\frac{\mu_b}{\mu_w}\right)^{0.14} \qquad \text{Eq. 6.3.2.} - 22$$

$N_{Nu} = Nusselt\ number \equiv \frac{hD}{k}$ Thus $N_{Nu,ln} = \frac{h_{ln}D}{k}$

Let us recognize: $\left(\frac{\rho\, v\, D}{\mu_b}\right) = Reynolds\ No.$ $\left(\frac{\widehat{C_p}\mu}{k}\right) = Prandtl\ No.$

Also, μ_b= viscosity of the bulk fluid
μ_w= viscosity of the fluid at the wall temperature

For laminar flow $\frac{h_{ln}D}{k} = 1.86\left(N_{Re,b}\ N_{Pr,b}\,\frac{D}{L}\right)^{\frac{1}{3}}\left(\frac{\mu_b}{\mu_w}\right)^{0.14}$ Eq. 6.3.2. – 23

For example, we talked about the correlation for highly turbulent flow under certain conditions and for laminar flow under certain conditions, 2 different expressions here.

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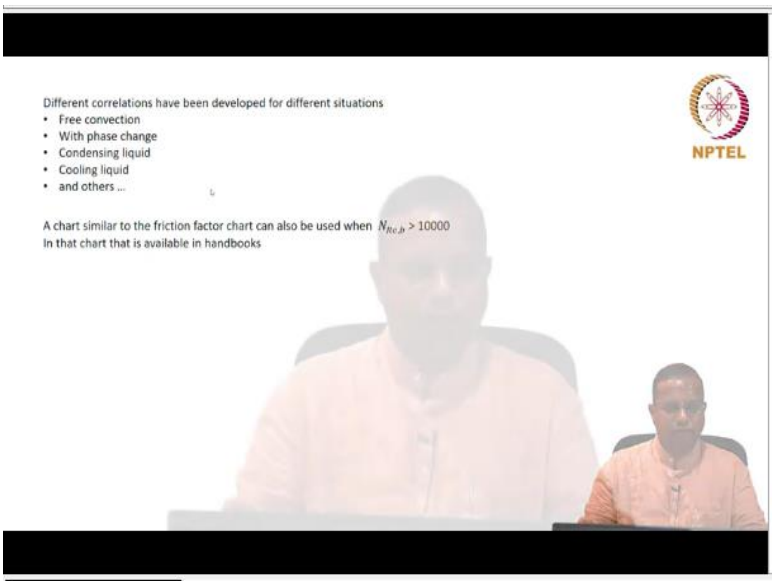

Different correlations have been developed for different situations
- Free convection
- With phase change
- Condensing liquid
- Cooling liquid
- and others ...

A chart similar to the friction factor chart can also be used when $N_{Re,b} > 10000$
In that chart that is available in handbooks

And I also mentioned in general that there are different correlations for different situations free convection has a different correlation, phase change has a different correlation, condensing liquid has a different correlation, cooling liquid has a different correlation and so on and so forth. So, different situations you pick up different correlations and then use to find the overall heat transfer coefficient.

And that is where we finished up the course. Hope that you found the course useful I hope that you also had fun. Do not worry about the mathematical complexity if you are not oriented towards mathematics. If you are then you had enough food for packing are interested in so on so forth. So, hope you had fun, I hope all of you had fun, if at all you need anything anytime, please feel free to write to me.

Okay, you know the communication details and email should be fine anytime, I wish you all the best. Let us sign off here, bye.