Modeling Transport Phenomena of Microparticles
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Lecture - 23
Detailed Routing (Part IV)

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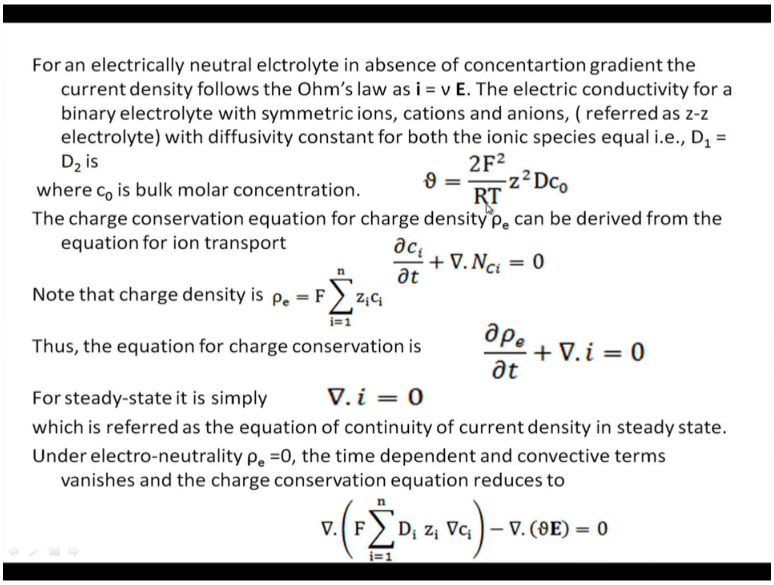

Now so if it is a situation where the fluid electrically neutral so here described now fluid electrically neutral and there is no gradient in ionic species so this is the Ohm's law i = Nu

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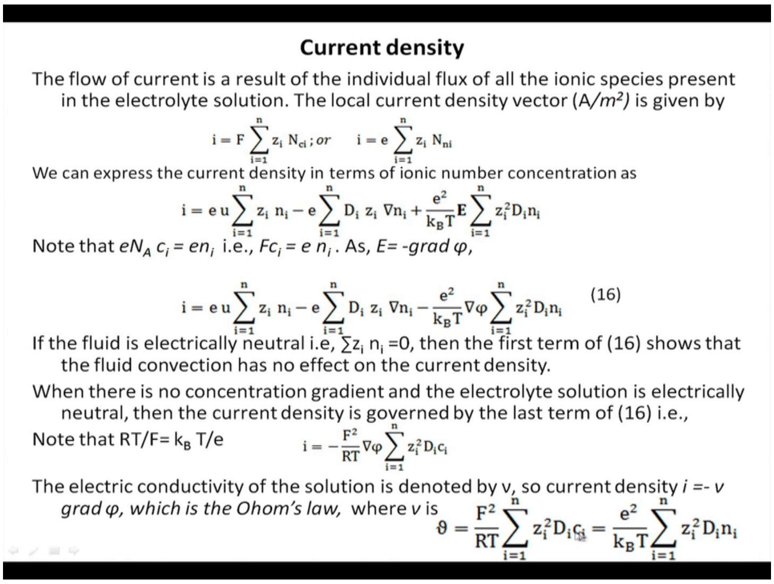

As we have derived before so and this zi square is the net number density of zi square is the net molar concentration of the electrolyte so this is see if I call this is this c0 is also can be referred mention or can be considered as a bulk value, now from these the current density equation we can derive the conservation of charge density and equation for the charge density can be derived this way.

So now charge density we have defined as Rho e equal to governed by this relation into zi is the molar concentration of ionic species so if I multiply with that and this is the relation so I get a situation the ionic flocks of the molar flocks of the ionic species So if it is multiplied with zi so which is nothing but the previous one, so we get a equation like this Del Rho by Del t + Divergence of i = 0, so this is referred as the conservation or charge transport equation.

Now if it is a steady state we have time derivative is zero so what we have is Divergence of i is zero at any point within the electrolyte medium, so this is also referred equation of continuity of current density in steady state, we can say this as the continuity equation for the current density. Now if we have the electrically neutral and time independent and convective terms vanishes is and the charge conservation equation reduces to this form.

Because what you have here this goes time derivative goes see if I take the Divergence in both side so you get a situation like this way okay, so these are the some important transport equation to characterize the Electrokinetics of ionized liquid.

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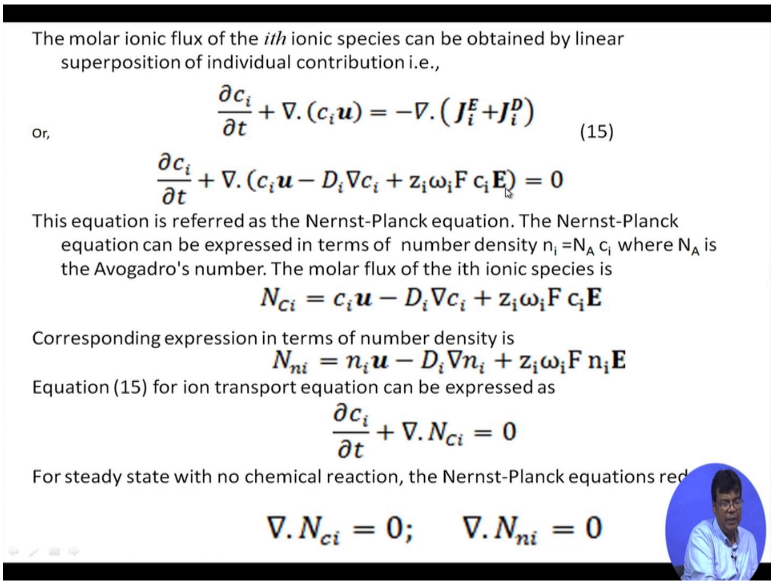

So as you could see the equation of ionic transport equation for ionic species is involving u, it is involving the E electric field.

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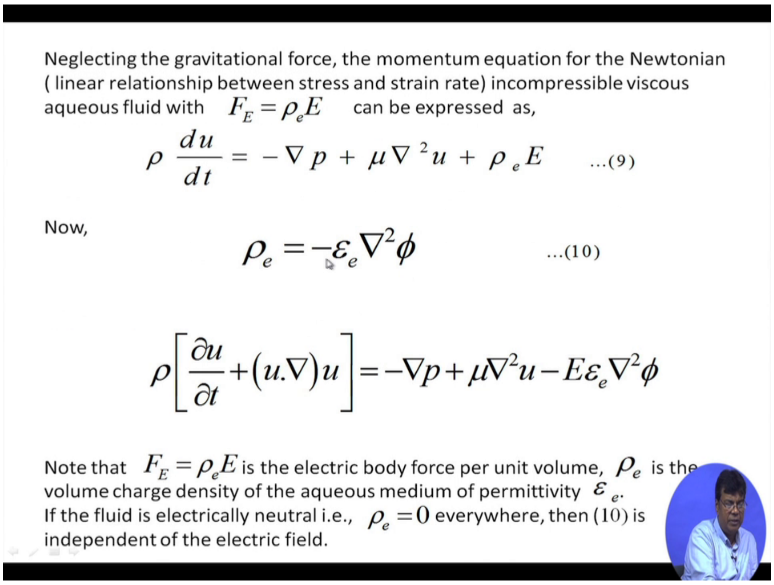

So this electric field is governed by this if you just look back electric field is governed by this Poisson's equation and this Poisson equation is also involved in the equation of fluid flow so that means all these equations are coupled so that means the solution of the or the form of the velocity or the ion distribution and the electric field are interrelated.

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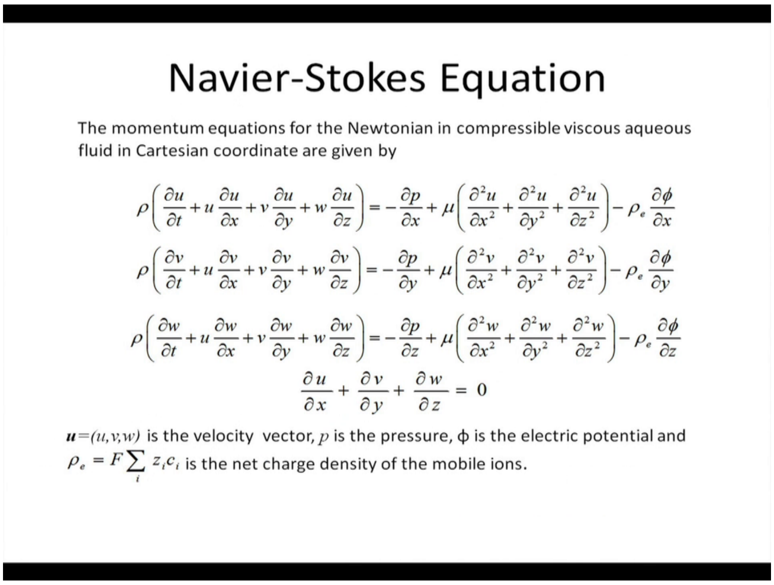

Now if I write this equation in a Cartesian co-ordinate form, the transport equations which we referred as the Navier Stokes equation for the incompressible Navier Stokes equation we get a situation like this. This is the electric body force stuff or the things are usual situation for usual Newtonian incompressible fluid flow equation, so if there is a pressure difference occurs and if there is a flow there will be a non zero pressure gradient and the continuity by this is the x momentum or u momentum equation this y direction, this is z direction so here we have three component of velocity.

And Rho e is a charge densities obviously Rho is not a constant also because it involves the molar concentration of the an ionic flocks which may vary when the space vary with x, y, z.

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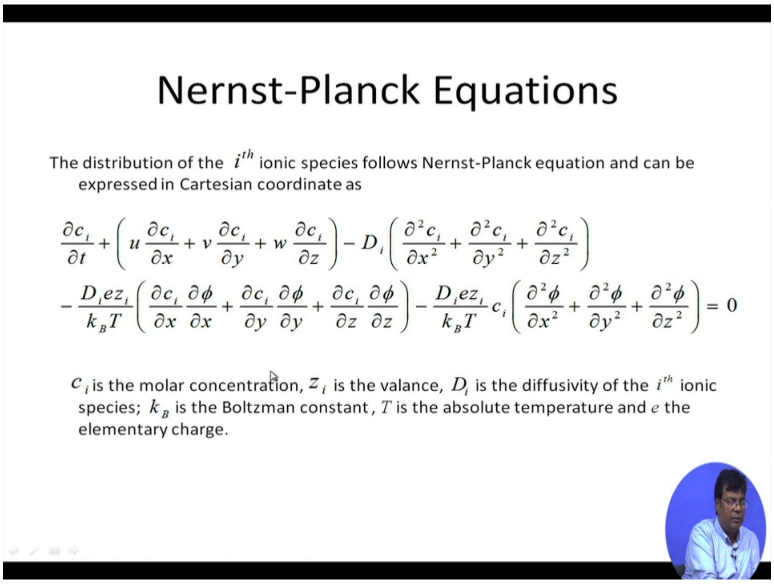

So the other equation the equation for Ion transport is referred as The Nernst-Planck-Equation. So Nernst-Planck- Equation for the ionic species is now can be expressed in Cartesian co-ordinate this manner okay now here we may have a number of ionic species so each ionic species will obey this equation and the valance is zi, so and once I get this ci at any point for all these s so no one can get the charge density Rho e.

And then one can write the equation so obviously this equation is related or depending on this equation of ion transportation equation is also referred the Nernst-Planck- Equation

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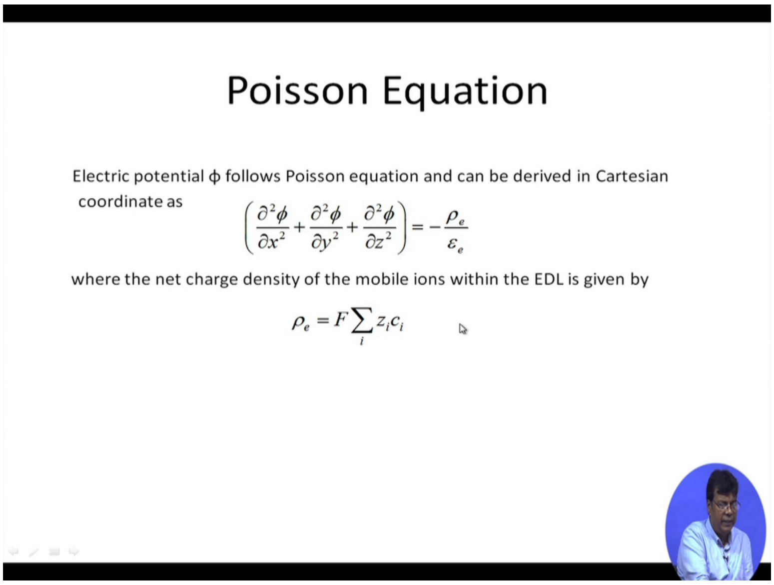

And this equation this set of equation are supplemented are by the Poisson equation for electric field which we have derived already, so what do you find that this is a linear equation of-course. But other equation see this equation are all nonlinear second order and quite complicated situation. So it is involving this kind of elliptic form because of this Laplacian and also it has a proclivity because of this kind of first order gradients.

So you have u dot Grad situation so this is a complicated and is also nonlinear so solving this set of equations are quite complicated situation.

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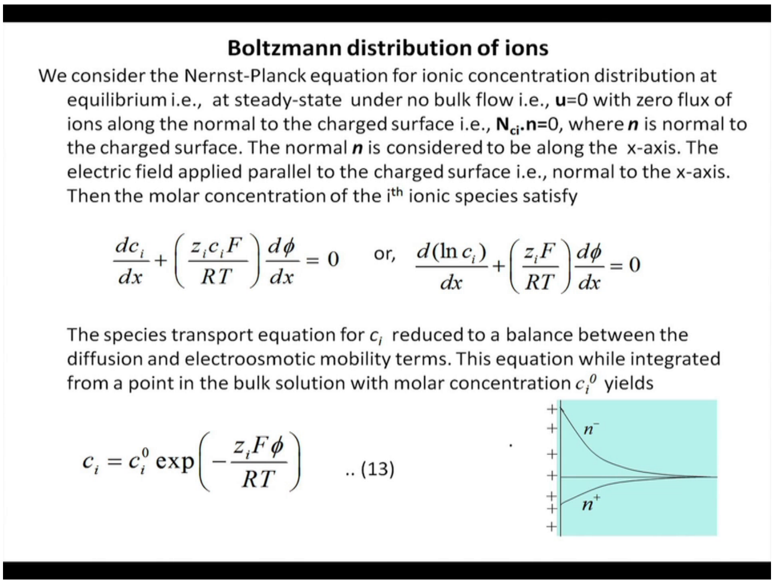

Now to simplify that so there are several ways one can simplify so one of the simple way is the considering a situation where we have the equilibrium situation that means the there is no flux of ions that means this is written wrongly.

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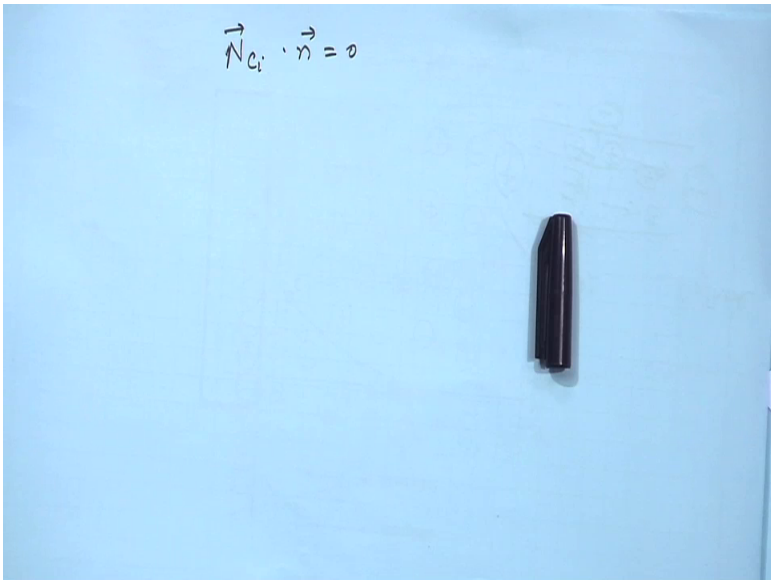

It should be Nci dot n = 0 so here it should be Nci dot n = 0 and in a steady state situation, so if I assume that ion flocks is zero ion flocks and you have the convective fluid velocity is zero okay and 0 flocks of ions if I assumed this kind of situation, so then we can reduce this Nernst-Planck- Equation to this form for any ionic species given by this way okay.

So that means if I have this is the normal direction is x direction here normal direction we are considering here is a x direction and this is a plane is x = zero plane so this is a surface so what do you have is ion flocks normal to this is zero and you have a electric field across this parallel to the surface so in this case we can write the Nernst-Planck- Equation is simplified form as this now this can be club or interrogated simplified to this form.

And we get an integral of this equation given by now this now this c i 0, we call the bulk concentration that means at x = 0 where education constant is taken care by this c i 0 where we measure these a electric potential is becoming constant or 0 because another thing is that electric potential can have a non zero value what if it is a constant, sure if we subtract from the electric potential because electric potential appears in a gradient manner gradient form.

So if we subtract a constant from the electric potential Phi so it satisfy the same equation equation as is as the Phi - Theta or Phi - constant Satisfy or the same equation by the Phi itself okay.

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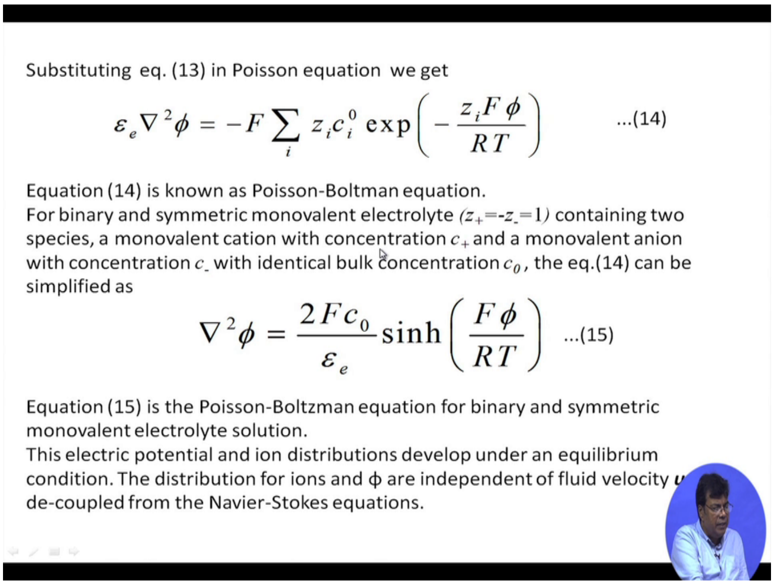

So the solution of the equation can be expressed in this manner now if I substitute the Poisson equation that means here we are considering a binary electrolyte and let us take monovalent electrolyte that means + equal to – z - = 1 so that means the valence is taken to the 1 so it is containing two species a monovalent cation with concentration and monovalent and anion with concentration with identical bulk concentration because if I assume the bulk electro neutrality.

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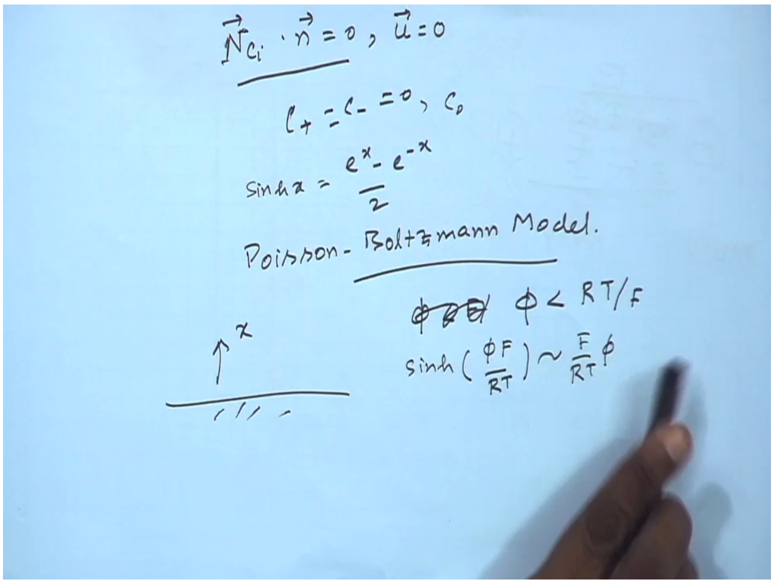

So what we should have is c + - c - = 0 so you have this okay. So c0 is the bulk concentration. If I assume so we can have a we can write this equation this form and so this Sin hyperbolic x = e power x - e to the power – x by 2, so this technique we apply this equation 14 it can be reduced to a equation like 15. So this equation is referred as the Poisson Boltzmann equation so again this is a nonlinear equation because Phi is involved over here in a nonlinear fashion.

But once I get the Phi I get the distribution of ions by this Boltzmann equilibrium Boltzmann distribution. So this model are based on few simplified assumption first of all what have assumed that the distribution of ions and Phi are in under an equilibrium condition and no bulk flow fluid flow is assumed so obviously here what we define that this is decoupled from the Navier Stokes equation.

So that means whichever way the fluid velocity is developed so this equation for electric field and the ions are independent of the Navier Stokes equation of the local fluid velocity okay. So that is the simplicity of the Boltzmann equation.

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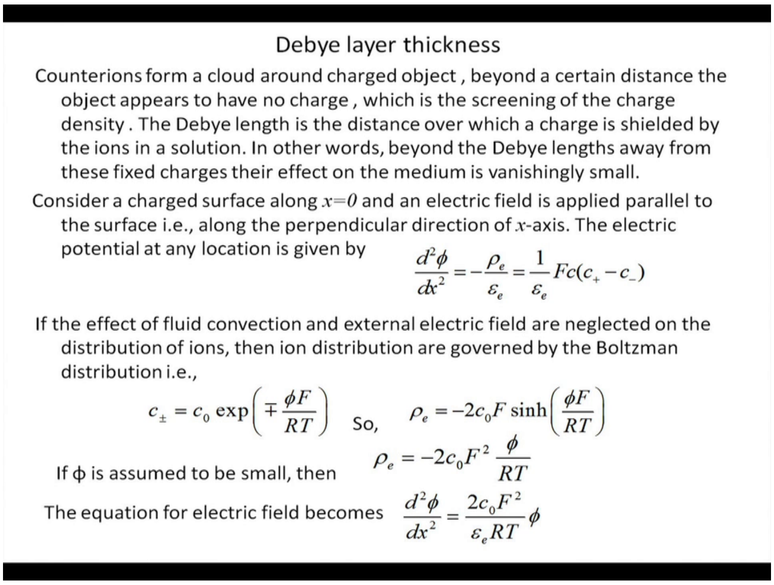

Now what will discuss about the Debye layer thickness now what we talked about that when there is a aqueous media which is in contact with solid surface so there will be a formation of diffuse layer stand layer and diffuse layer totally called as Debye layer so now this phenomena is also called the screening that means you have a situation where the surface charge has been screened by the Debye layer formation.

Now we would like to measure the screen length so that means what we can say is a Debye layer is such a length scale and beyond which the, this charge density has no effect on the fluid okay. Now so Debye length is a distance there is the way we can define Debye length is the distance over which it charges sealed it by the ions in a solution in other words beyond the Debye length away from the charges their affect on the medium is vanishingly small.

So when if we consider a situation Only One dimension does means here you have the x is this direction so what we can write the this equation from here we can write as this is a Poisson equation so d2 phi by dx2 equal to charge density by Epsilon e, so this is written as this now if I assume that the ions are obeying the Boltzmann distribution which is governed by this equation and show the charge density becomes – Phi F by RT.

Now here we make a assumption we assume that the Phi is quite small okay, if Phi a small smaller than F by RT, no Phi is smaller than RT by F, so that means what we can do is we can approximate the sin hyperbolic (Phi F by RT) is becomes (F by RT Phi) okay. So if I do this approximation if we assume Phi is to be small so in that case what a get that Rho e can be simplified this equation can be simplified to this form.

So this is a linearization so where is this is the linearized Poisson Boltzmann equation is governed by this equation is also called Debye approximation which will talk little bit later subsequently.

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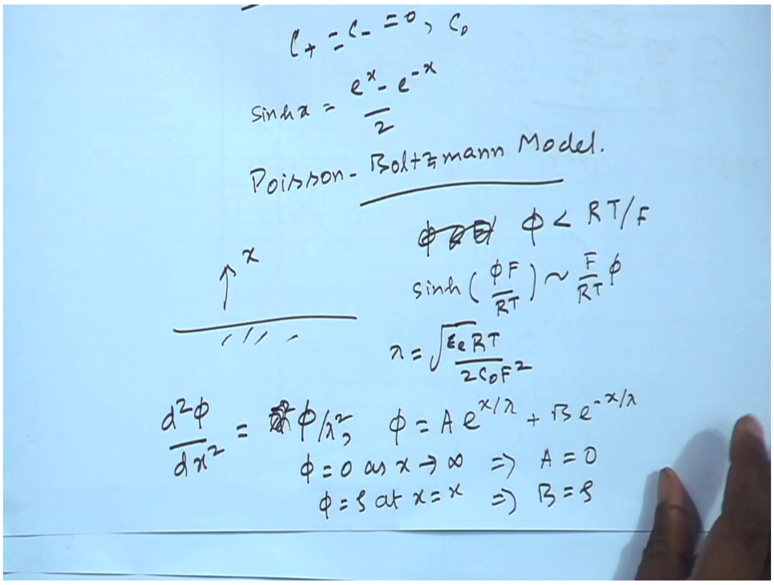

Now we have the differential equation d2 Phi by dx2 = 2c0F power 2 by Epsilon 0 RT Phi, now we define length scale say Lambda which is equal to root over Epsilon 0 RT by 2 c0 F power 2 Epsilon 0 is the permittivity, so if I define a length scale like this or some parameters Lambda so we can write now this equation as the d2 Phi by dx2 = Lambda square Phi. So the solution is Phi = A e to the power here it is the Lambda one, so this will be the inverse way.

So this is -2 so Phi by Lambda, so -2 so e to the power x by Lambda + B to the power –x by Lambda, so Lambda to the power -2 or Phi by Lambda square okay. Now the conditions or whatever is given is Phi = 0 as extends to infinity, because the electric potential is a bulk it is a neutral whatever the value I can take subtract from this Phi and you can take Phi = 0 and whatever the constant value because Phi approaches the constant so this implies that A is 0 Now if you have Phi = Zeta at x = 0 so you get B = 0 so Phi = Zeta means you have a constant for potential on the surface x = Zeta

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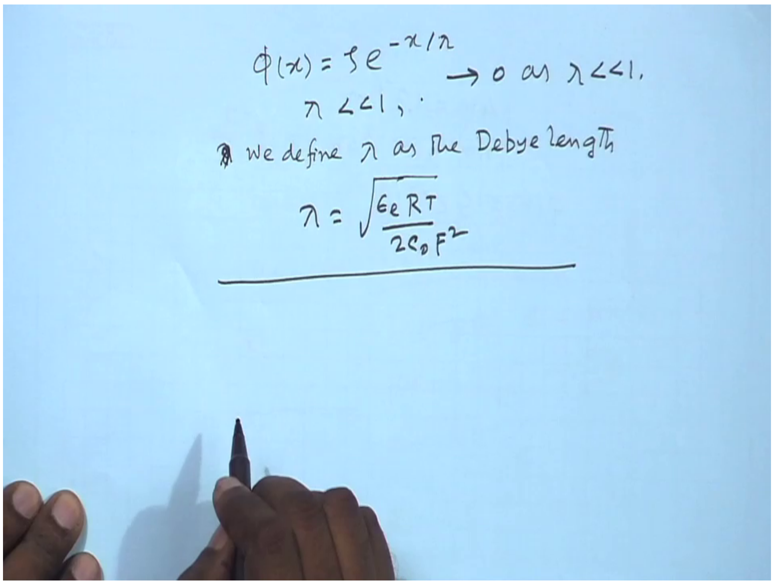

So from here we get an equation as this form we get an equation that is Phi, now Phi (x) = Zeta e to power – x by Lambda okay. So Phi now becomes Phi (x) = Zeta e to power – x by Lambda now this shows that if when Lambda becoming small so that means you have this becoming large x by Lambda so if Lambda is many, many times less than 1, so by this term is tending to 0 as Lambda many, many times less than 1, so that means beyond the Debye length so Lambda with define.

So far we not defined anything with define Lambda as the Debye length, so Lambda how you are defined is Root over Epsilon 0 RT by 2 c0 F square, so is that the Debye length is depending on the bulk molar concentration of the electrolyte should given an electrolyte with the permittivity of Epsilon e. We can find out the Debye length which gives an estimate that up to which, the up to which length the charge which is situated at the surface screened up to which length okay.

So we can say that x becoming larger than the Debye length we will have the charge density tending to 0. Now so far we have discussed about the transport equations, So now we have to see the boundary conditions.

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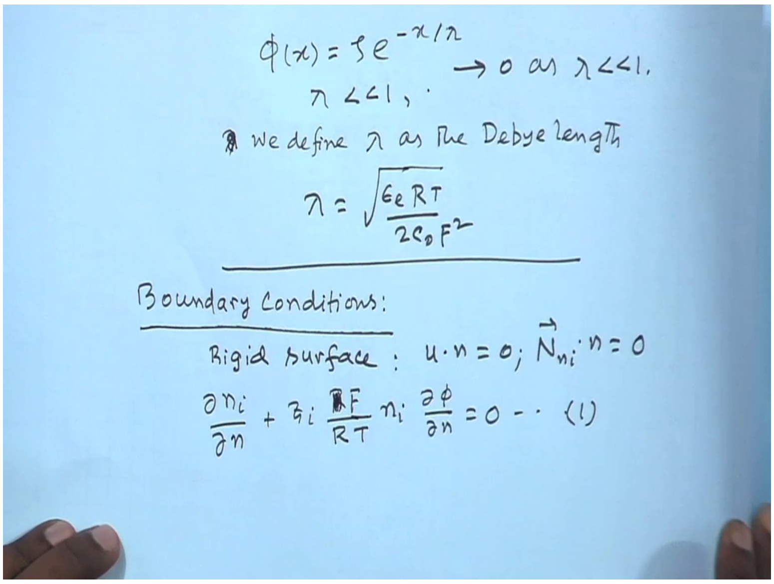

Which we can imposed the boundary conditions on this kind of to analyze the flow problem because we have the partial eventual equation as you could see here you have a second order elliptic type of equations so that means all the boundary conditions for x, y, z, are to be given so always we have a Laplacian operator for elliptic type of form so this demand that the boundary condition I need to be prescribed in order to get a solution for this kind of equations.

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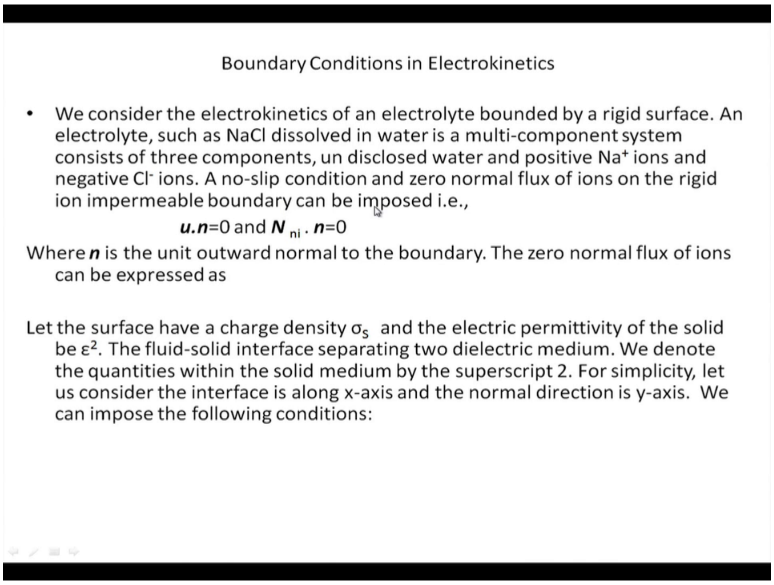

Now how the body conditions are developed or governed, now boundary condition means we have a rigid surface over which say we considered ion impermeable rigid surface so rigid surface which is ion impermeable and written so that means what we have is no normal flux of the ion across the surface and the velocity across the surface is zero, so N here we are is the measuring or N is denoting here is a unit outer normal to the boundary.

So we have these two conditions u dot n = 0 and N ni dot n = 0 so this N ni = 0, the rigid surface so no normal flow and N ni this flocks across the surface, so 0 flocks on the surface. So this gives the related condition gives you Del ni by De n + Zeta i F by RT ni Del Phi by Del n = 0, so this is the two conditions or combinly I can write as equation 1. Now if we have Del ni by Del n is zero so that is now gradient in electric field so we can simply write Del ni by Del n = 0, so this again will give you the Boltzmann distribution.

Now let us consider a surface charge on the surface rigid surface you have a surface charge density, so let the surface service charge density is Sigma s and the electric permittivity of the solid be Epsilon 2 .

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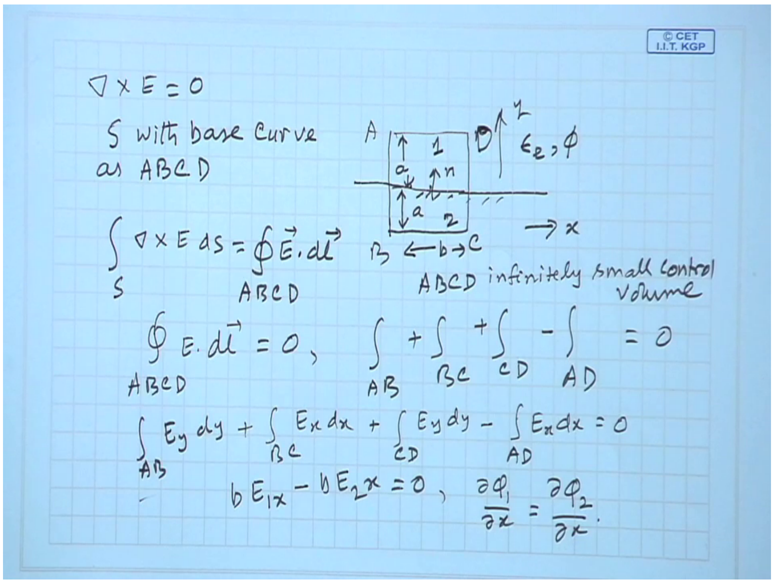

Now we have a situation say here so which is the interface between two or over which the liquids or fluid like show latest call this liquid which has Epsilon e and the potential is Phi is now we know that Delta cross E = 0, everywhere so we construct a control volume or arbitrary area is in two dimension ABCD let is take this ABCD okay, arbitrary area which contains the interface.

And now we construct a surface is with base curve base curve as ABCD say cylinder or close surface with Base curve as ABCD Delta cross E = 0 everywhere. So if I now apply the Stokes theorem Delta cross E, s can be written as the counterintergration or integration over these curves ABCD of E dot dl, dl is the line element on this. So what we have is integral ABCD E dot dl = 0. Now this is the surface in now let this distance is A height this is also we take asymmetrically.

So this is A and this is B, so when we call so this is equal to integral of over AB + BC + CD - AD. So it will be a some direction now when I am integrating this E dot dl, so the line element here it is this is x axis and perpendicular is y, so here it is Dy and so that means you have here integral over AB E y dy, the component this plus integral over BC E x dx + integral over CD E y dy - integral over AD E x dx = zero. Now these two are will be the equal and opposite.

So what we left over is integral this is because we assumed that these are infinitely small, so ABCD is a infinitely small control volume, so the on the surface we neglect any change of this Ex, Ey components so from here I can write now if here this is within a solid zone and if I called denote this as the superscript 2 or subscript 2 and this is with subscript 1, so we can right now when I am in on BC so this is b into E 1x and this is will be b into E 2x = 0.

So this gives you Del Phi 1 by Del x = Del Phi 2 by Del x, so this is the continuity condition of the electric field at the interface so the next one will carry forward to the next lecture.