Modeling Transport Phenomena of Microparticles
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Lecture - 29
Two-dimensional EOF

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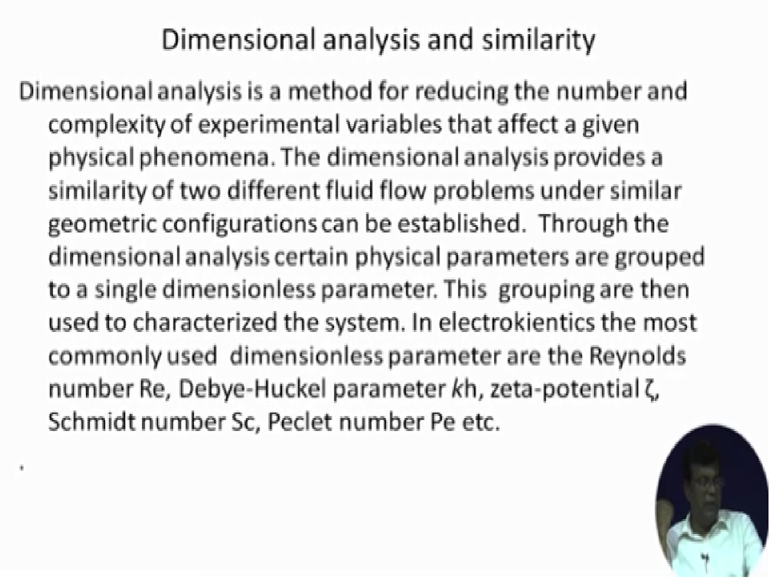

Dimensional analysis and similarity

Dimensional analysis is a method for reducing the number and complexity of experimental variables that affect a given physical phenomena. The dimensional analysis provides a similarity of two different fluid flow problems under similar geometric configurations can be established. Through the dimensional analysis certain physical parameters are grouped to a single dimensionless parameter. This grouping are then used to characterized the system. In electrokientics the most commonly used dimensionless parameter are the Reynolds number Re, Debye-Huckel parameter *k*h, zeta-potential ζ, Schmidt number Sc, Peclet number Pe etc.

So we were talking about EOF by the Nernst Planck model for fully developed Nernst Planck equation and fully developed EOF, in a slit-micro channel, now we have derive the equations know this dimensional analysis is we have to perform now. What is the importance of dimensional analysis and similarity is a little bit described over here now see, the dimensional analysis basically what we to do is a grouping of some parameters. There are individual parameters so this individual parameters.

Speed up of that group to a single sometimes a non-dimensional parameter so which characterizes the flow or the electro kinetics of the electromagnetic transport for this situation. Now, for example in the hydrodynamics we have the known Reynolds number. So, similarly for the electrokinetics the most commonly used at the Reynolds number, Debye-Huckel parameter, Zeta potential, Schmidt number and Peclet number etc., now for that through this parameter values we can have a correspondence between two phenomena in a similar configuration.

So that is the importance of the dimensional analysis.

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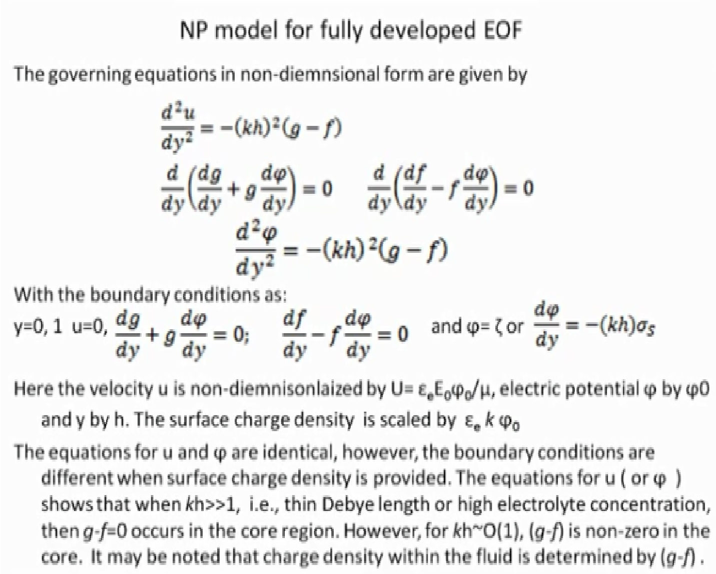

NP model for fully developed EOF

The governing equations in non-diemnsional form are given by

$$\frac{d^2u}{dy^2} = -(kh)^2(g-f)$$

$$\frac{d}{dy}\left(\frac{dg}{dy} + g\frac{d\varphi}{dy}\right) = 0 \qquad \frac{d}{dy}\left(\frac{df}{dy} - f\frac{d\varphi}{dy}\right) = 0$$

$$\frac{d^2\varphi}{dy^2} = -(kh)^2(g-f)$$

With the boundary conditions as:

y=0, 1 u=0, $\frac{dg}{dy} + g\frac{d\varphi}{dy} = 0;$ $\frac{df}{dy} - f\frac{d\varphi}{dy} = 0$ and $\varphi = \zeta$ or $\frac{d\varphi}{dy} = -(kh)\sigma_S$

Here the velocity u is non-diemnisonlaized by $U = \varepsilon_e E_0 \varphi_0/\mu$, electric potential φ by $\varphi 0$ and y by h. The surface charge density is scaled by $\varepsilon_e \, k \, \varphi_0$

The equations for u and φ are identical, however, the boundary conditions are different when surface charge density is provided. The equations for u (or φ) shows that when *k*h>>1, i.e., thin Debye length or high electrolyte concentration, then *g*-*f*=0 occurs in the core region. However, for *k*h~O(1), (*g*-*f*) is non-zero in the core. It may be noted that charge density within the fluid is determined by (*g*-*f*) .

Now in previous class we have derived the Nernst Planck model or fully developed EOF. Where the velocity which is parallel flow, we are considering this is U is along the axis of the channel or along which the electric field is applied and this is the distribution of the ions so we have taken the monovalent binary ions. So G and F for the concentration of the ions. So this satisfied the set of equations ordinary Differential Equation for that matter.

And along with these boundary conditions are governed by this issue as we stated before. The boundaries are Y = 0 and Y = 1. These are the Y = 0 is lower wall Y = 1 is upper wall so on the wall, we have zero fluid velocity zero normal flux so normal flux condition given by this way. Along with either constant Zeta potential or you can have a constant surface charge density. Here is Kappa is the inverse of Devilier thickness know dd is in driving this equation.

We have non-dimensionlaised the velocity by this capital U which is a similar to the small Smoluchowski velocity but potential is Phi 0. Which is the scale for the electric potential and E0 is the applied electric field and Phi scale by Phi e0 thermal potential RT by F which is about point zero or two point or you can say 26 millivolts or point two six volt and Y we have scaled by the height of the channel and the surface charge density is normal scaled by this Epsilon e Kappa Phi 0.

Now if you look at this equation so what is at the governing equation? What you find that these equations are governed by the parameter Kappa h and the Zeta potential for the service charge density parameters Sigma s. So individually we do not have to specify the height of the channel or the diffusivity because here these are the convective transport of ions are all neglected and also the conviction terms in the fluid flow equation is also neglected.

So this is simply governed by the Kappa h. So if I describe the Kappa and Kappa means the Devilier thickness again the Devilier thickness is also governed by the electrolyte concentration and the permittivity of the electrolyte and so on, which is already been defined before so and other things like temperature and real gas constant. It is a constant volume, but fluid to fluid you can have a different Viscosity, different permittivity.

So these parameters are all group together to form is Kappa h and this is U small Smoluchowski velocity. Now we look into this equation. What do you find that if Kappa h is very large? So Kappa h large means the h by Lambda is large in other words the Debye length is very small Lambda is Small. So that case what we find that G - F is occurring so that means outside the code of the channel.

We can have an electro neutrality of the solution. And also these two equations are U and Phi equations of the same form but they have different boundary conditions. So but if I choose the boundary conditions is Phi = Zeta and see the one main thing is that for the electric potential only the gradient is important. So even if I define say some Phi - Zeta so I can assume Phi = 0 on the both the wall so this form of the Phi are change because of this same equation.

If I redefine Phi - Zeta so U and Phi have the same solution provided you have Phi = 0 if I consider. So but if I choose Kappa h is the order 1, so that means Lambda the Debye length is not ready in thin so that case we can have G - F to be non-zero. Now one way is to solve this set of equations. Which is a strictly speaking is a nonlinear boundary value problem because you have the two point boundary Y = 0 and one.

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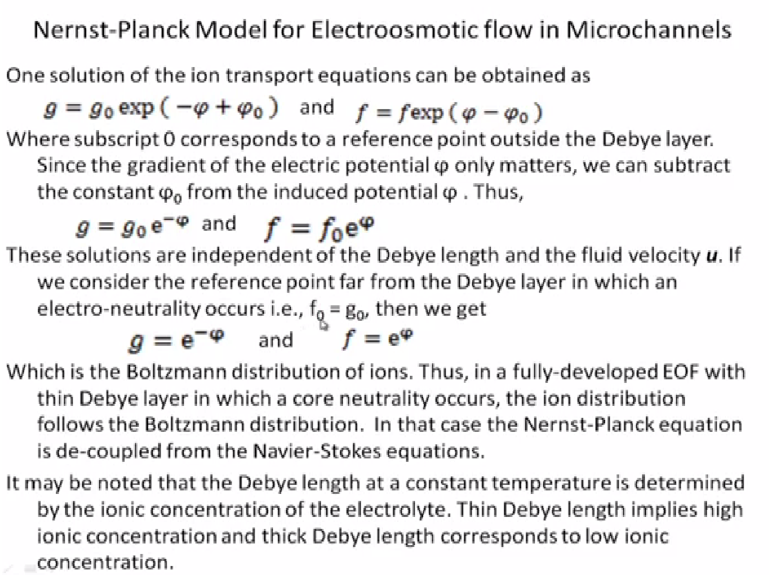

Nernst-Planck Model for Electroosmotic flow in Microchannels

One solution of the ion transport equations can be obtained as

$$g = g_0 \exp(-\varphi + \varphi_0) \quad \text{and} \quad f = f \exp(\varphi - \varphi_0)$$

Where subscript 0 corresponds to a reference point outside the Debye layer. Since the gradient of the electric potential φ only matters, we can subtract the constant φ_0 from the induced potential φ . Thus,

$$g = g_0 e^{-\varphi} \quad \text{and} \quad f = f_0 e^{\varphi}$$

These solutions are independent of the Debye length and the fluid velocity ***u***. If we consider the reference point far from the Debye layer in which an electro-neutrality occurs i.e., $f_0 = g_0$, then we get

$$g = e^{-\varphi} \quad \text{and} \quad f = e^{\varphi}$$

Which is the Boltzmann distribution of ions. Thus, in a fully-developed EOF with thin Debye layer in which a core neutrality occurs, the ion distribution follows the Boltzmann distribution. In that case the Nernst-Planck equation is de-coupled from the Navier-Stokes equations.

It may be noted that the Debye length at a constant temperature is determined by the ionic concentration of the electrolyte. Thin Debye length implies high ionic concentration and thick Debye length corresponds to low ionic concentration.

So one can compute this solve this one but were the easy way is, that we can I have to integral for the Nernst-Planck equation for this one dimension case. Then we solve for is in form like this. Where we consider subscript zero a reference point outside the Debye layer, so these two integral satisfy the equation for G and F. Now the gradient of Phi is important. So I can redefine the induced electric potential in this case as Phi – Phi 0.

So if I do that I can get g = go e - Phi and f = f0 e Phi these two shows that they are independent of Kappa h. So, whatever the choice of Kappa h the ionic concentration is invariant and it is a similar to the Boltzmann distribution. Also now I can choose that if we have a situation. That outside the Debye layer you have a electroneutrality the reference point if I choose in such a way that electro neutrality has occurred.

So that case I can have the f0 = g0 which is basically the mole fraction. So at the equilibrium on the code. Where there is a electro neutrality is established. So I can write the solution g = e - Phi and f = e Phi the scaled two is the mole fraction of the cation and anions. So clearly these are governed by the same as the Boltzmann distribution of ions. So they also found the solution of the Nernst-Planck equation.

So far this is fully developed case what I can say is the convicted transport has no effect. If we have a code neutrality is established. So the Debye length of upwards here say always we always mention about the high large Debye length, thick Debye length & thin Debye length. So when we say the thin Debye length so we have to understand that it is a highly electrical concentration of the electrolyte is high, anybody say thick Debye length so we can that implies that concentration of electrolyte is low.

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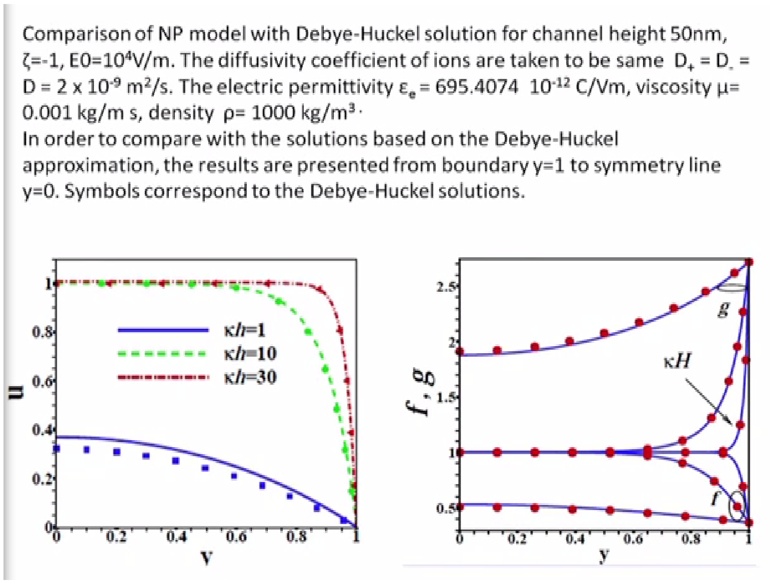

Comparison of NP model with Debye-Huckel solution for channel height 50nm, ζ=-1, E0=10^4V/m. The diffusivity coefficient of ions are taken to be same $D_+ = D_- = D = 2 \times 10^{-9}$ m^2/s. The electric permittivity ε_e = 695.4074 10^{-12} C/Vm, viscosity μ= 0.001 kg/m s, density ρ= 1000 kg/m^3.

In order to compare with the solutions based on the Debye-Huckel approximation, the results are presented from boundary y=1 to symmetry line y=0. Symbols correspond to the Debye-Huckel solutions.

So now if we make a update the solution for this Nernst Planck equation and now we compared with the Debye-Huckel solution which is obtained before so we get a situation of form like this. So the Debye-Huckel solution and the Nernst Planck solutions whichever is obtained if we make a comparison with is two so we get a comparison of this form, now what we defined is that when the Kappa h is quite low.

So in that case we find a situation where there is a difference in the solution so here to the sake of comparison we have taken zero to one, zero is the symmetry line of course when we are solving the Nernst Planck equation we have not taken any imposed any symmetry. What we have done is here that we have taken -1 and 1 as the domain so that means a wall are end -1 and 1.

And so zero is the symmetry line on the channel and that is how the Debye-Huckel solution is obtained. So what we find that Debye-Huckel solutions are okay at thinner Debye length. So that means when electrolyte concentration is high Kappa h are say greater than one so we get a good

comparison with the Debye-Huckel solution but if we have the Debye layer thickness are comparable with the channel height. So that means Lambda k = 1, which mean Lambda = h.
To this case basically what is happening is overlap of the Debye layer. So, h is the half height of the channel. So, that means the Debye layer what is occurring on the upper wall adjacent wall so they are overlapping so there we may not have a electro neutrality of the where did the code itself. So that is expected so that is why we have a slight difference from the Nernst Planck computer, Nernst Planck solution at the Debye-Huckel solution.

Another thing is that interesting thing here Kappa h is large we get Plug like type so that means there is a very the code of the channel we have a constant velocity, at constant velocity is nothing but the Smoluchowski velocity. Here of course Zeta potential is taken to be -1 which is means Zeta potential is scaled by Phi 0 thermal potential. So this is the same as the Smoluchowski velocity should be at one and this is the fluid property.

Now we see the distribution of mole fraction, so that means in the code where is Kappa h is larger Kappa h is one so this are the two mole fraction, so that means in the code there is a g - f is one zero. Charge density at any point within the fluid is proportional to g - f because that is the net amount of concentration of the ions, so if g - f is non-zero so that means the fluid is electrically non neutral.

So what we find this Kappa h when it is a small value so we get it g - f is non-zero whereas in this situation so Kappa h is large so that means the Debye length is thin or electrolyte concentration is high, what we find that G and F causer coinciding with each other so that means you have a zero charge density in the code is established only a little bit jump ss there a difference is there near the wall or near the Debye layer.

So at this is Y equal to what is the wall over which the Debye layer forms, so close to the Debye layer we have a large value of g - f outside the Debye layer you have a zero charge density. So also the ions distribution is not very much for at all because ion distribution is not affected by the fluid convection the solution whatever we have shown upwards here we have taken a Debye-

Huckel approximation so that way the Phi whatever is obtained is not the same as the Poisson-Boltzmann case.

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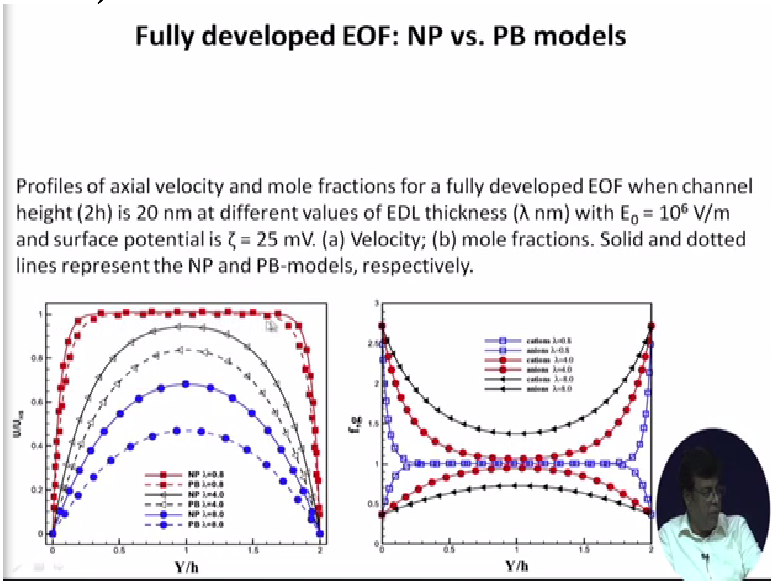

Fully developed EOF: NP vs. PB models

Profiles of axial velocity and mole fractions for a fully developed EOF when channel height (2h) is 20 nm at different values of EDL thickness (λ nm) with $E_0 = 10^6$ V/m and surface potential is $\zeta = 25$ mV. (a) Velocity; (b) mole fractions. Solid and dotted lines represent the NP and PB-models, respectively.

Now if I compare with the instead of Debye-Huckel approximation if I take the full Poisson Boltzmann equation that is nonlinear Poisson Boltzmann equation for the electric field and if your compute that nonlinear equation and compare with this solution of the differential boundary value problem we have described that is what is referred as the Nernst Planck model or the NP model.

So what we defined that it is they just the same they just my coinciding with each other so there is even see the Debye length is Lambda point eight, so where the channel height is twenty Nano meter. So point eight we find the constant code flow that was within the code Y is zero at the two but that two boundaries where, so outside the Debye layer quickly approaching the velocity again here Zeta is -25 should be -1 this is a dimension form 25 mV, which is nothing but the thermal potential?

So I get a value as saturation value as one or the constant core velocity but when I increase the love the thickness of the device is increasing in other words the electrolyte concentration is reducing. We find a situation is a parabolic flow type of parabolic like a first flow is established between the two parallel plates channel and which get a situation this floor resembles to the public profile which appears in the person so this is the correct plug like profile.

It is very important in many microfluidic devices and also what I can say is that they can regulate the floor because it is just a function of e0 that external applied electric field and other thing as we discussed feels like that you see the code neutrality is not established when Lambda is large, when Lambda = 8 or core nano meter you get the G and F profile or even this two cuts so obviously G - F is non-zero within the core.

But as we increase the electrolyte concentration or decrease the thickness of the developed show codified is that we could utility is establishing the G - F becoming 0.

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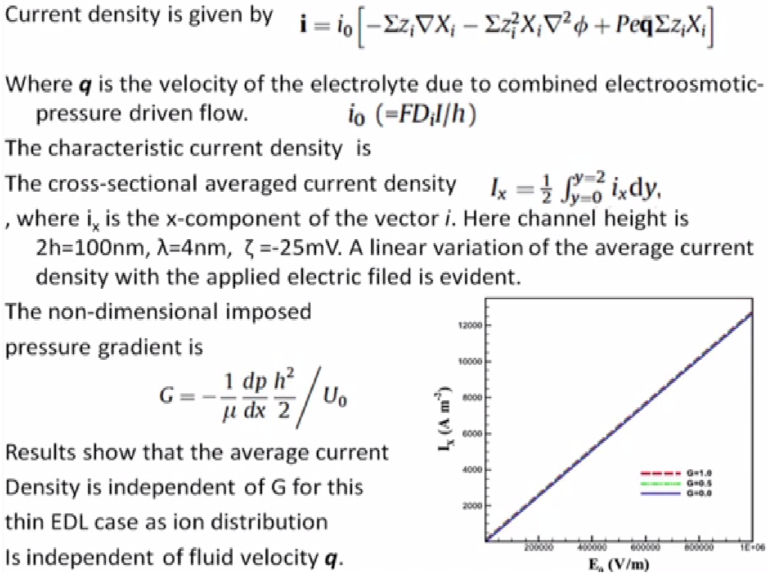

Current density is given by $\mathbf{i} = i_0\left[-\Sigma z_i \nabla X_i - \Sigma z_i^2 X_i \nabla^2 \phi + Pe\mathbf{q}\Sigma z_i X_i\right]$

Where $\boldsymbol{q}$ is the velocity of the electrolyte due to combined electroosmotic-pressure driven flow. i_0 $(=FD_i I/h)$

The characteristic current density is

The cross-sectional averaged current density $I_x = \frac{1}{2}\int_{y=0}^{y=2} i_x \mathrm{d}y$,

, where i_x is the x-component of the vector i. Here channel height is 2h=100nm, λ=4nm, ζ =-25mV. A linear variation of the average current density with the applied electric filed is evident.

The non-dimensional imposed pressure gradient is

$$G = -\frac{1}{\mu}\frac{dp}{dx}\frac{h^2}{2}\bigg/ U_0$$

Results show that the average current Density is independent of G for this thin EDL case as ion distribution Is independent of fluid velocity $\boldsymbol{q}$.

Now current density can be obtained, as we discussed before also for the Poisson Boltzmann model say where the current density this vector is given by this way so if I take this characteristic current density as i0 which skills that i know this person is becoming a non- dimensional. Because we have by the non-dimensional not initialized the variables here Q is the velocity v0 considered now Q is the fluid velocity and excise the mole fractions all this here introduce one parameter dear this is Epic number.

Now Beckley number, Beckley number appears which we have not define before so Beckley number appears because of the diffusivity of the ions and the fluid velocity so basically the Beckley number which is governed by.

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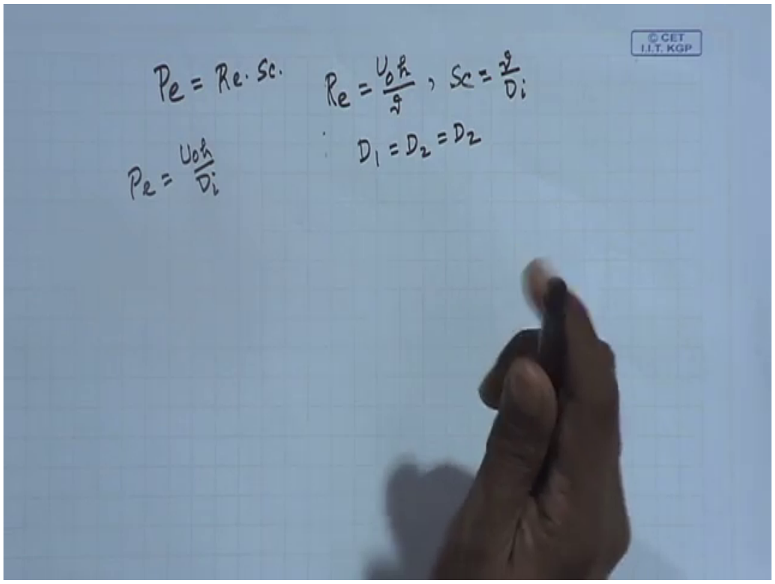

If I right p, where q is the electrolyte due to combined Electroosmotic pressure driven flow. So if I what is the Reynolds number this is basically here is the U0 is the velocity and this is length scale h and the Nu which is the kinematics viscosity and Smith Number is nothing but Nu by dy, where dy is the molecular diffusivity of the y, so here we have taken that di to be Sim, if you considered the binary electrolyte and if you considered D1 = D2 = D2.

That is the diffusivity of the all the ions or Sim in that case we find that this number this is non dimensional number Beckley number becomes u0 h by di so this is basically the ratio of the adjective transferred of the ion by the molecular diffusion transport. So this is the number occurs, so Electroosmotic flow one thing to remember is that this quantity that this non dimensional Reynolds number is quite small because it is very small in the micro meter range Uo is also small.

But this can be quite large because di is very small for the bio colloids, bio fluids and all so di is like it into the - 10 or - 9 factor so in that way this product RDSC can be of order one so if RDSC this Beckley number is neglected this contribution of this term as no use. So basically the ion density which is governed by the concentration of the concentration gradient as this is the mobility of the ions we have non dimenionlized, this equation we have before.

And the convective transport of the ions, now this time can be zero this last up provided you have a zero electro neutrality or Beckley number is very small go through the solution whatever the equations we have solved. So we define this Ix is a cross-sectional average current density here what you have done is a combined flow of Electroosmotic and procedure went through so that means there is a constant pressure gradient is also applied along the axis of the channel.

Which is measured by this non dimensional effect of G, now if we compute or if you plot the average crossover is current density here it is written in dimensional form submitted meter square against the voltage electric field voltage drop on electric field should I find that says first follow the case is G = 0, so that inspired Electroosmotic flow, so you get a linear variation so this linear variation suggest that it is transferred have very little effect.

And also it for the shows that if I write this G that is the pressure difference is not changed now here we have taken the Debye length as 4 nano meter and 2h is 100 nano meter so they are far apart so that means a core neutrality is established so this we may have the Zi Xi zero within the core. So you get a linear solution. But if we have Lambda point?

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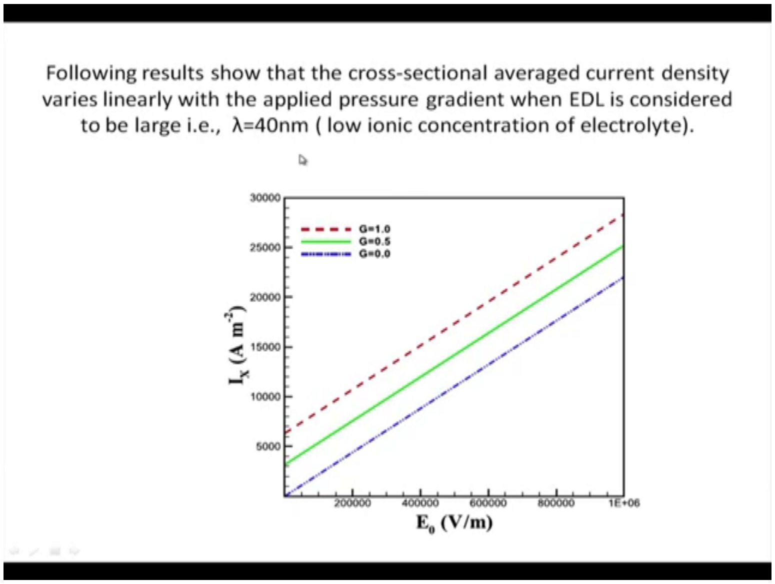

Following results show that the cross-sectional averaged current density varies linearly with the applied pressure gradient when EDL is considered to be large i.e., λ=40nm (low ionic concentration of electrolyte).

Lambda large 40 nano meter, So here within the core of the channel V electrically neutral so we find that effect of G. Effect of G is now quite evident from here linear increment in the current density so this is how we can measure the Electroosmotic pump current density through a slit channel on fully developed if.

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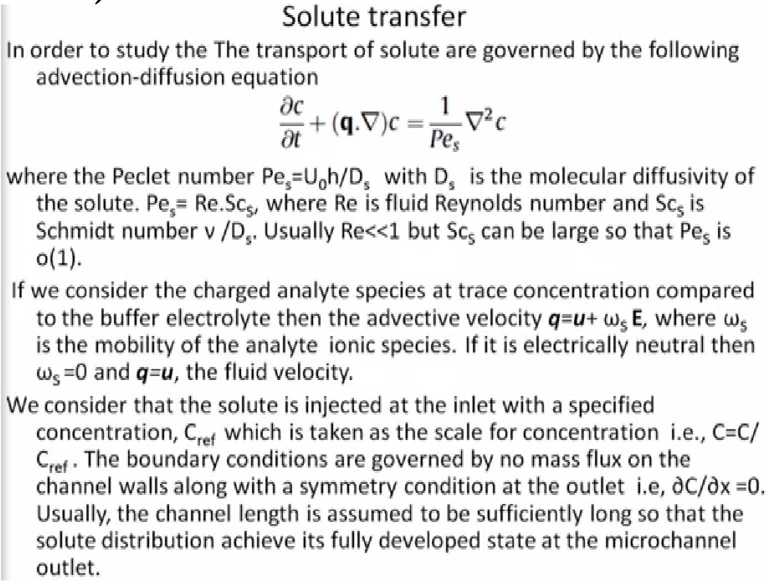

Solute transfer

In order to study the The transport of solute are governed by the following advection-diffusion equation

$$\frac{\partial c}{\partial t} + (\mathbf{q}.\nabla)c = \frac{1}{Pe_s}\nabla^2 c$$

where the Peclet number $Pe_s=U_0h/D_s$ with D_s is the molecular diffusivity of the solute. $Pe_s= Re.Sc_S$, where Re is fluid Reynolds number and Sc_S is Schmidt number ν /D_s. Usually Re<<1 but Sc_S can be large so that Pe_S is o(1).

If we consider the charged analyte species at trace concentration compared to the buffer electrolyte then the advective velocity $\boldsymbol{q}=\boldsymbol{u}+ \omega_S \mathbf{E}$, where ω_S is the mobility of the analyte ionic species. If it is electrically neutral then $\omega_S=0$ and $\boldsymbol{q}=\boldsymbol{u}$, the fluid velocity.

We consider that the solute is injected at the inlet with a specified concentration, C_{ref} which is taken as the scale for concentration i.e., $C=C/C_{ref}$. The boundary conditions are governed by no mass flux on the channel walls along with a symmetry condition at the outlet i.e, $\partial C/\partial x=0$. Usually, the channel length is assumed to be sufficiently long so that the solute distribution achieve its fully developed state at the microchannel outlet.

Another important aspect in Electroosmotic flow is easily transferred so that means a micro channels are connected to reserved words. So what you need is transferring the solute from one reserve it to the other, so salute can be a neutral salute that is electrically neutral or it in this concept stress concentration means its concentration is too low that he does not change the electric activity of the or electrokinetics of the buffer electrolyte.

So if we consider the solute concentration is very low so it is referred as a stress concentration so the other properties of the electrolyte are independent of the presence of solute. Now the solute transport equation governed by this advection diffusion and if it is a charged and there will be electromigration so this equations advection diffusion and electromigration as we have described before so this is the one the Peclet number which is just fine before.

And DS is molecular diffusivity of the solute now this Q this is the can be a combination of the if it is a neutral salute so we do not have this second term. So it is cross voting with the or advection velocity is that invite the fluid velocity background electrolyte velocity so we have the adventives velocity q = u + Omega is e, Omega is mobility of the analytic ionic species if it considered a charged solute.

So the solute transport equation and so is governed by this equation so if I take this is out Ws, omega is zero so what we find that if I know the value of u at every point. We know the solution you one can solve the this equation advection diffusion equation this is the diffusion term, this is the advection term and get the distribution of the solute at any time.

Now to see the investigate the how the solute is travelled, suppose we considered a portion of the channel so at the inlet we are injecting the solute with a fixed concentrations. Which we called as the sea reference which is the scale for the solute concentration, so that means non dimensional concentration is defined c equal to say some c bar = c y, c reference at the boundary conditions are governed by nomads flask on the channel was so that is nothing but here channel walls.

We are taking as normal is y, through y axis that is the Y = 0 and Y = 1, so what we can impose the condition is Del c Del I = 0 on the channel walls and the outlet we can have a symmetry. So that means the symmetric distribution so you can have the gradient or fully developed situation for the solute distribution, we can have the gradient Del c Del x = 0 of the solute at the outlet.

So this is a elliptic portion of this equation and also we have the this is a parabolic situation hyperbolic we would not say because u is known and this because of the presence of this term if we have this Ps is quite large. So that means we have the diffusivity touts is negligible but that you will not be the case for this situation PS is always of order one.

That means it is a kind of elliptic and parabolic combination, so it in since it is a second derivative of C so you know all the four non due conditions and also initial condition. So we assume that initially there are some solute C0 is within the channel.

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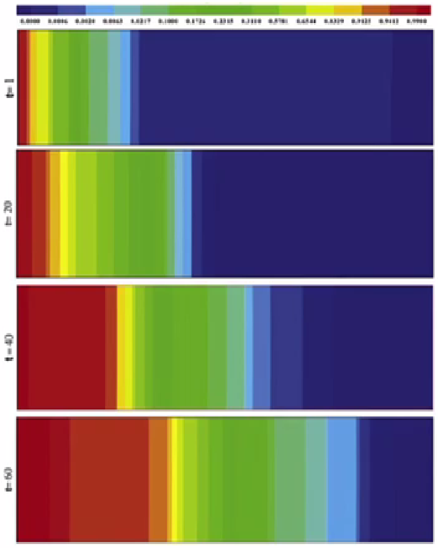

Following figure shows the distribution of solute in the slit channel with charged walls under an electric field E0 $=10^5$V/m when 2h=100nm, λ=8nm, ζ = -25mV with $Sc=\nu/D_s=7692.31$.

The average bulk flow rate is 1.595 x10^{-3} m/s at $E_0 = 10^5$ V/m, and the corresponding Peclet number is 3.574. This shows that the transport of solute is diffusion dominated.

Now if we solve we get the distribution of the solute with time is governed by this equation. Here we are together external electric field applied electric will it take to do a 5 volt watt meter height of the channel has 15 and 2 Hs is 100 nano meter, Lambda is 8 nano meter, and Zeta is 25 mV, taken the diffusivity of the solute in such a way that Smith number this is this number is given by the way, the Peclet number is comes to be 3.54.

Because the average bulk flow is which determines the Reynolds number so there is – 3, but Peclet number comes to be 3.54 this distribution shows that the solid transfer is mostly occurring to the diffusion mechanism. So we initially we are injecting the solute this rate at the high concentrations in the solid at the inlet and it is transported along the X direction by Electroosmotic flow and by the molecular diffusion.

So with time this is the so what I find out from this result that the solute EOF mixing in the micro channel is very slow process and its most diffusion mechanism so this is the bottleneck of some situations where we need a rapid mixing of the solute may be charged or uncharged species so we need to consider how to add and hence the mixing of the solid so that I will continue with the next thing will continue in the text lecture.