Environmental Geomechanics

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Lecture No. 41
Contaminant transport through porous media-III

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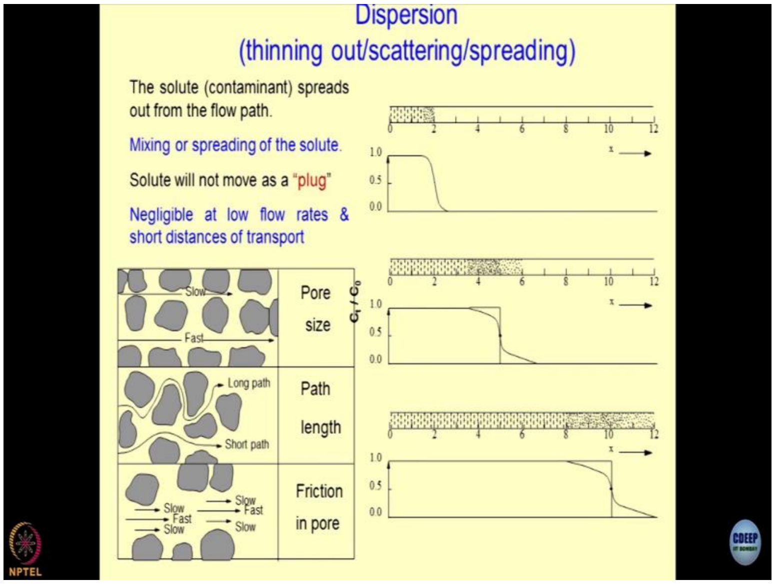

Dispersion
(thinning out/scattering/spreading)

The solute (contaminant) spreads out from the flow path.

Mixing or spreading of the solute.

Solute will not move as a "plug"

Negligible at low flow rates & short distances of transport

Let us talk about the third mechanism of contaminant transport, which is dispersion. So, I mean, the literal meaning is getting dispersed is not thinning out of something spreading scattering. So, here you have a plug of certain concentration. And now, because of the flow of water, what is happening, the concentration over a distance gets spread out. That means here the concentration is dropping down.

So this is a concentration profile at this end, you have a higher concentration at this, and you have a low concentration on the x-axis. So C_t/C_0 at this point is 1. C_t/C_0 at this point, is 0. This is a step gradient now, as this concentration front moves, what happens? There is a spread out of the concentration, and C_t/C_0 becomes substantial what is the logic when you try to study the dispersion phenomena we use these type of models.

Which tell you how dispersion phenomena is taking place. This is a micro mechanism associated with the dispersion mechanism. The analogy is similar to the pipe flow; if I asked you to draw the velocity profile in the pipe flow, you could draw it maximum at the centre and at the two ends because of the wall friction or the friction of the pipe the velocities are less the same analogy I can use over here.

So, if you consider the velocity contrast within the sample as far as the pore size is concerned, the pores which are bigger would allow you allow the migration of water to be faster as compared to the pore which is quite close to each other. There could be a concept of the path length. Also, the difference between this discharge velocity and the friction velocity remember, so, the short path is normally straight, and the torturous path is going to be the longish path.

And then, of course, we talk about the friction in the pores. So, these are the 3 mechanisms which are normally used to define the dispersion process. So, the velocity is going to be more in the central portion of the port as compared to the place where the water is in contact with the soil grains because this is where the friction is getting mobilized and the velocity of the flow is going to be less so what causes dispersion.

Ultimately, the dispersion is because of the contrast of the velocity in different layers of the sample. So, imagine a situation where within the pores, you have a velocity contrast. So, this is going to result in the dispersion process. Similarly, the long and short part distances within the pores are also going to create dispersion phenomena and of course, the pore size. If pore sizes are not uniformly distributed, the dispersion is going to be prevalent. Is this part okay?

It so happens that in case of the clays and the sands, normally, we do not talk about the dispersion, because the seepage velocities are going to be extremely small and dispersion gets rolled out. **"Professor - student conversation starts"** Sir why at the bottom dispersion is least it is not the bottom dispersion is least you are talking about this figure it is getting reduced. No, it is not that is the just to show you that if the pore distance is too much, the velocity is going to be more discharge is going to more as compared to the smaller. Of course, the second logic could be the path length third logic could be the friction.

So, at the ends of the pipe, there are though friction is also there, because of the pipe surface and that path length contribution is also there. So, both factors are contributing. As we go above the friction is getting reduced only the path factor is there. So, see friction is going to be constant in the pipe flow is it not means, at the bottom, the friction will be shared on the bottom. Basically, this is the contact between the fluid and the pipe where the friction is mobilizing correct. **"Professor - student conversation ends."**

Now, within the fluid, the central portion of the fluid is migrating faster as compared to the portion, which is in contract with a pipe, and that part is understood. So, this contrast in the velocity itself is going to create dispersion or the variation in the pore sizes or the variation in the flow path. So, these are the three models which you create to study the dispersion phenomena. So, in short, the dispersion is because of the change in or let us say gradient in the velocity which gets created in the pore system, and the answer or the reasons could be 123. This is how we are modelling it.

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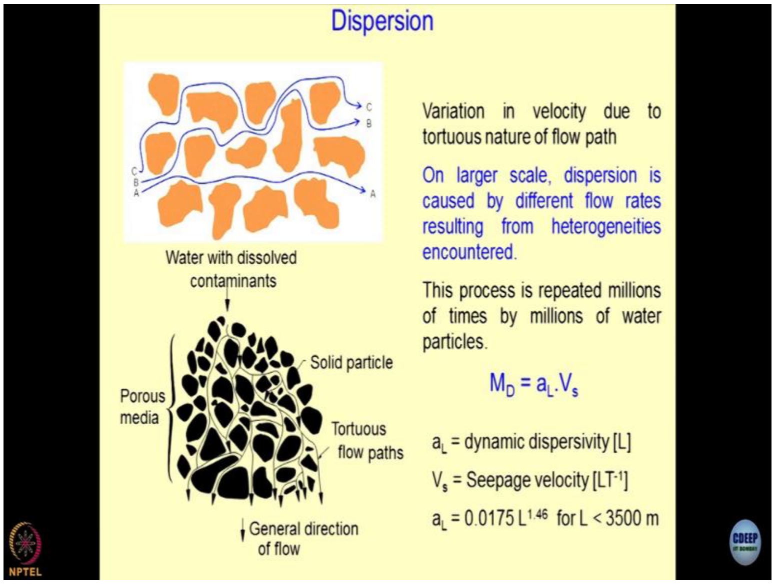

Dispersion

Variation in velocity due to tortuous nature of flow path

On larger scale, dispersion is caused by different flow rates resulting from heterogeneities encountered.

This process is repeated millions of times by millions of water particles.

$$M_D = a_L . V_s$$

a_L = dynamic dispersivity [L]

V_s = Seepage velocity [LT^{-1}]

$a_L = 0.0175 L^{1.46}$ for $L < 3500$ m

So, from this point onwards this is the poro mechanics, which starts, I am sure you must have heard a name of the poro mechanics in geomechanics it is becoming a very advanced subject, where the pore size analysis is being done by using the most sophisticated instruments, because now the realm of the discussion you must be realizing is Intra pore, inter pore. So what is happening inside the pore is becoming more interesting and more important.

So, I will be talking about how to do the pore structure modelling subsequently, because as you said some time back what is the importance of the porous media. So, porous media is defined by its core structure. And then the question is how to quantify the pore structure, how to differentiate between the pore structures. So, in today's world, everything is being done, and I will discuss with you how it is done.

So, this picture just shows you how the solid particle and the fluid interaction takes place, what is the torturous path and what is the direction of the flow and truly speaking how the porous media is defined or how it is modelled is this part okay?. So, when we talk about the dispersion, we use the coefficient $M_{D,}$ and this is equal to another coefficient we call it as a dispersion coefficient in the lateral direction multiplied by the seepage velocity.

So, a_L is the dynamic dispersivity, V_s is a seepage velocity, and a_L is a term which depends upon the flow path. These are empirical relationships which are used for modelling the dispersion phenomena but as I said, because when the flow takes place to the compacted soils, the seepage velocity is going to be extremely small is it not? and hence M_D term becomes insignificant tortuous path I think you understand the seepage path and the general direction path is the discharge path.

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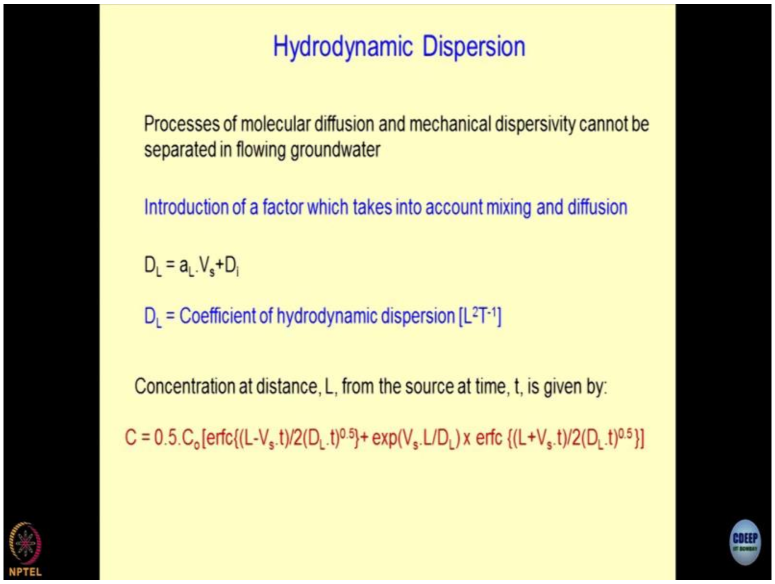

Hydrodynamic Dispersion

Processes of molecular diffusion and mechanical dispersivity cannot be separated in flowing groundwater

Introduction of a factor which takes into account mixing and diffusion

$D_L = a_L.V_s+D_i$

D_L = Coefficient of hydrodynamic dispersion [L^2T^{-1}]

Concentration at distance, L, from the source at time, t, is given by:

$C = 0.5.C_o[\mathrm{erfc}\{(L-V_s.t)/2(D_L.t)^{0.5}\}+ \exp(V_s.L/D_L) \times \mathrm{erfc}\,\{(L+V_s.t)/2(D_L.t)^{0.5}\}]$

The fourth process through which the contaminants might migrate in the porous media is hydrodynamic dispersion. So, hydrodynamic dispersion is a process where some mechanical activities required to trigger or to accelerate the molecule diffusion. A good example would be the potassium permanganate, which I added to the water column in the glass. If I let it happen on its own, it will take a lot of time.

A better way would be you stir it with a spoon. So, what will happen, the entire thing will become uniform colour, or uniformly concentration in no time. So, what hydrodynamic dispersion does is it gives you the mechanical effect as far as the distribution of the concentration is concerned in the system. I hope you can realize that in a porous media, hydrodynamic dispersion cannot be valid is this okay.

But hydraulics people when they are talking about some discharge coming and entering into another reservoir of water let us say when you are disposing of the sewage in the sea. So, what is done is you take the pipe and flush out all the sewage into a big reservoir. So, in this case, hydrodynamic dispersion is valid, but as far as geomaterials are concerned hydrodynamic dispersion is ruled out again. This is the governing equation which deals hydrodynamic dispersion $D_L = a_L \times V_s + D_i$. So, D_i is again the diffusion in the Free State. So, D_L is the coefficient hydrodynamic dispersion the units remain the same L^2/T.

L is the distance T is the time, and if you solve this equation, you will get C_t/C_0 error functions, and there are exponential terms and if you substitute the values of time at a given time what is the value of the concentration of the contaminants or at a distance. So, if you see the L, L would be the distance of the point where I want to find out the concentration, this can be obtained by using this type of expressions. So, these are simple models which are used for obtaining the concentration of contaminants in the porous media.

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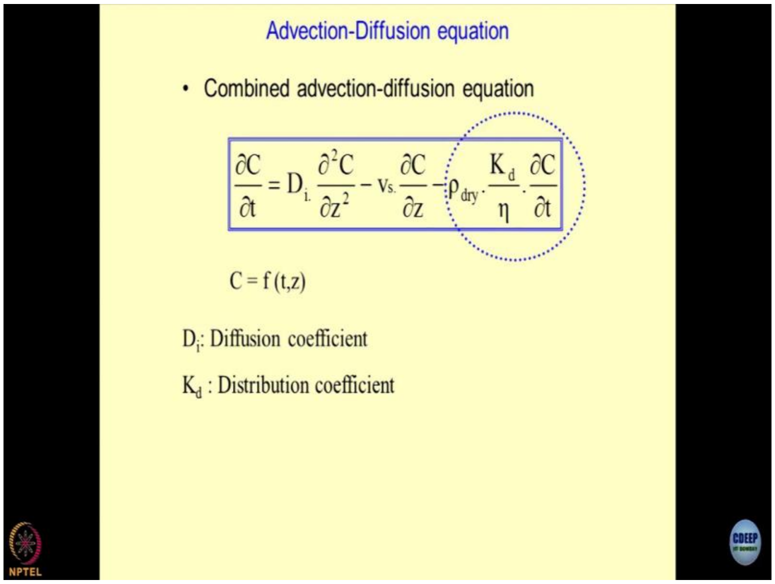

Advection-Diffusion equation

- Combined advection-diffusion equation

$$\boxed{\frac{\partial C}{\partial t} = D_{i.}\frac{\partial^2 C}{\partial z^2} - V_{s.}\frac{\partial C}{\partial z} - \rho_{dry}.\frac{K_d}{\eta}.\frac{\partial C}{\partial t}}$$

$C = f(t,z)$

D_i: Diffusion coefficient

K_d : Distribution coefficient

Now, if I club all these things together and as a geotechnical engineer, I will be more interested in advection-diffusion equation because as I said molecular diffusion, molecular dispersion and hydrodynamic dispersions are ruled out in our context, this is how this equation looks like. So, this is a clubbed form of advection and diffusion process we call this as one-dimensional ADE. One dimensional why because you are talking in terms of only in terms of z-axis.

ADE corresponds to advection Diffusion equation rate of change of concentration with respect to time is diffusion coefficient multiplied by $ð^2C/ðz^2$, this is the second Fick's law I hope you understand, - seepage velocity into ðC/ðz what is the component this is V×C= mass flux. So, this is because of the seepage velocity the rate in change, rate of change of concentration along the length of the sample. This coefficient K_d is the distribution coefficient, which defines the sorption desorption phenomena.

Which we are talking about, eta is the porosity of the soil mass or the porous media, ρ_{dry} is the dry density of the porous media, $ðz/ðt$ is the rate of change of concentration with respect to time. So, this equation is one-dimensional ADE. Now, if you do a bit of mathematical jugglery, you can obtain the K_d parameter. So, there are several ways of doing the analysis of this equation, and this is where the practice of environmental geomechanics is important. Normally you will come across the situation where you are doing monitoring let us say.

So, suppose if I dispose of the waste at a given point and I will like to measure what is the concentration of the chemical species at a certain x, y, z and t. So, I can put sensors over there I can drill the bore logs, I can collect the water sample, I can take out the soil sample, and I can establish what is the concentration at this point. In other words, I can know the value of C at a given time and z by doing experiments or by doing field studies.

And I can substitute it there I have to compute Vs seepage velocity which is not difficult to do. If I know discharge velocity, I can divide by the porosity, and I can get the seepage velocity. Now, what is going to be difficult is how to obtain the K_d parameter, because that is a new subject in itself. So, when you ask this question to yourself how to obtain K_d, which is sorption desorption phenomena, then we have to enter into absorption desorption, which is a sort of chemical characterization of soil contaminant system.

Another way of looking at this equation would be if I can measure K_d parameter, if I know the porosity, if I know the dry density of the porous media, if I know the seepage velocity if I know the diffusion coefficient, I can substitute these terms in this expression and what I can obtain is $ðC/ðt$. So, the rate of change of concentration with respect to time and what I have to do is I have to obtain the rate of change of concentration with respect to distance.

So, again you have to follow the time series. Is this part okay? Now, one more interesting thing from this equation which can be observed is if I take this term on the left-hand side, what happens with this expression becomes $ðC/ðt. (1+ K_d) \times \rho_{dry}/\eta$. So, $1 + \rho_{dry} \times K_d/\eta$ is known as retardation parameter which I had shown you at this place. If you remember, we were talking about.

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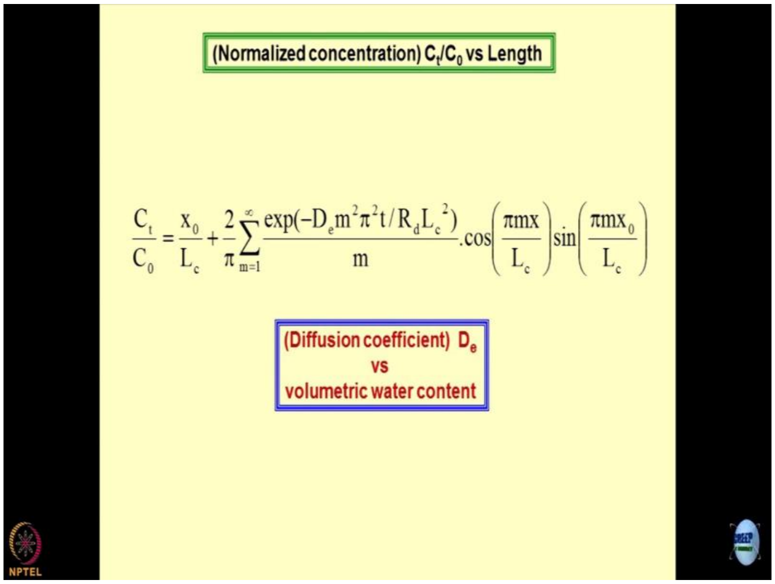

(Normalized concentration) C_t/C_0 vs Length

$$\frac{C_t}{C_0} = \frac{x_0}{L_c} + \frac{2}{\pi}\sum_{m=1}^{\infty}\frac{\exp(-D_e m^2\pi^2 t/R_d L_c^2)}{m}.\cos\left(\frac{\pi m x}{L_c}\right)\sin\left(\frac{\pi m x_0}{L_c}\right)$$

(Diffusion coefficient) D_e
vs
volumetric water content

The R_d parameter over here is it not? So, this R_d is equivalent to $(1+\rho_{dry}) \times K_d/\eta$ all the countries which are into nuclear activities. I hope you understand nuclear activities you understand what do they do? They have to have researchers who are going to solve these expressions for various reasons. I hope you got the point. It is easy to run a reactor by using a nuclear source of power.

But the question is variable to dispose of the atomic waste nuclear waste got it. So, suppose you have an atomic power plant, you have to solve this equation to make sure that this is going to be the zone in which no rehabilitation should occur number 1, if at all this zone is becoming too limited, because of the encroachment of the land by the people. And suppose in a country like Japan, where space is extremely less how to restrict the zone is a challenge which a geotechnical engineer has to take.

And this is where I would like to use barrier systems. Do you remember we were talking about containment and if I cannot contain it, what I should do, I should remediate it decontamination? So, everything is getting interlinked now, and that becomes an interesting problem modelling, giving a solution to the cause of something. Is this path clear? But, I am sure you must realize the difficulties also, which I told you because the parameters are not known.

Now, the question is if I am dumping the waste over here, and if I have to find out what is happening over here, I have to keep on taking the samples from different places of the soils. At what radial distance and what depth how many samples will take out. Sampling is not going to be easy. And imagine the disposal depths are in few hundreds of meters 200 meters 300 meters 400 meters. So, what is going to happen? You will be having a zone of influence which might be running in a few kilometres.

So, a big challenge is how many samples should be taken and hence what type of subject we are going to know use to answer this question, reliability analysis. So, what is the reliability of the sampling? What is the reliability of the data which you are generating by lab tests or the field test, how reliable the data is, which is going to be corresponding to real-life situation now, this is the practice of environmental geomechanics. I hope this point is clear to all of you.

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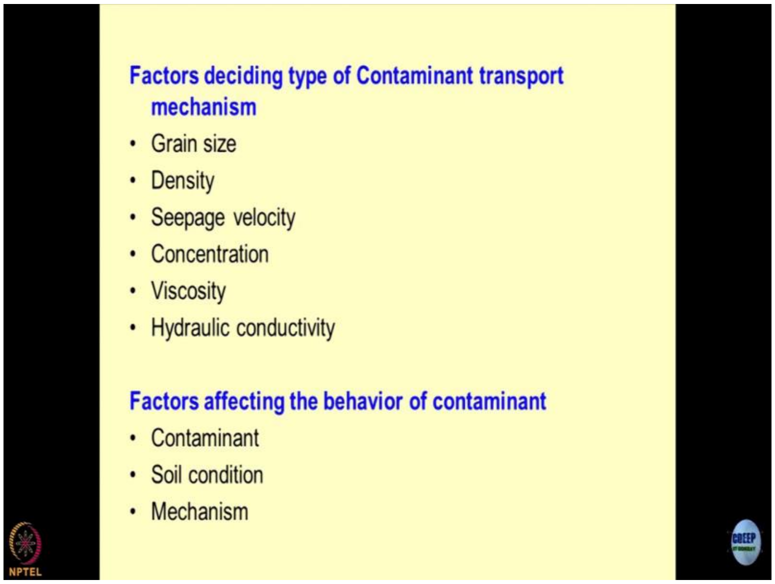

Factors deciding type of Contaminant transport mechanism

- Grain size
- Density
- Seepage velocity
- Concentration
- Viscosity
- Hydraulic conductivity

Factors affecting the behavior of contaminant

- Contaminant
- Soil condition
- Mechanism

What are the factors which influence the contaminant transport mechanisms, the grain size of the porous media? Yes **"Professor - student conversation starts"** In my again call in my college again, they were using some Langmuir model like equations to find this desorption sorption parameter, and then they can put it into the I am very happy that you are much ahead of that time will come I will discuss so these are all known as sorption desorption isotherms. We will talk about that. **"Professor - student conversation ends."**

So, the isotherms which are you talking about are the sort of breakthrough curves which will give you the K_d parameter; we will discuss this. So, let me start with the factors which are responsible for contaminant transport in porous media. First is grain size, seepage velocity is a direct function of the grain size distribution, the texture is a function of grain size, pores structure pores distribution is a function of grain size, density, seepage velocity, the concentration of the chemicals, viscosity of the contaminants, hydraulic conductivity. So, these areas per the porous media are concerned if you include all these terms, the porous media is defined. Now, what are the parameters which will be affecting the contaminants themselves? So, type of contaminant and its concentration clear and its activity, whether it is active, non-reactive, radioactive, non-radioactive. So, the type of contaminants, type of soil condition.

So, this is a big matrix which people are trying to solve another thing is contaminant transport is going to depend upon the mechanism. Just now, we have studied four mechanisms advective, diffusive, dispersive and hydrodynamic dispersion. So, you have to see what mechanism is controlling the contaminant transport, and there are few regulatory numbers, which I will be discussing can be utilized to establish what type of contaminant transport is occurring in the porous media

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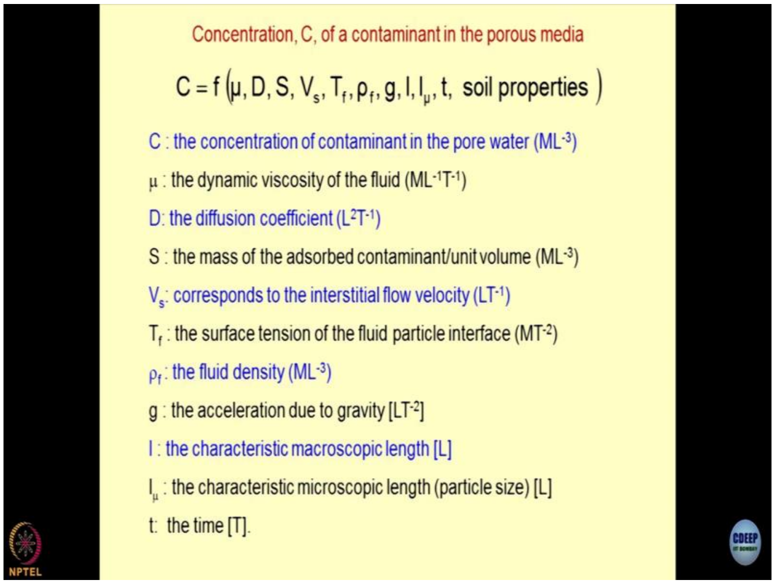

Concentration, C, of a contaminant in the porous media

$$C = f\left(\mu, D, S, V_s, T_f, \rho_f, g, l, l_\mu, t, \text{ soil properties}\right)$$

C : the concentration of contaminant in the pore water (ML^{-3})

μ : the dynamic viscosity of the fluid ($ML^{-1}T^{-1}$)

D: the diffusion coefficient (L^2T^{-1})

S : the mass of the adsorbed contaminant/unit volume (ML^{-3})

V_s: corresponds to the interstitial flow velocity (LT^{-1})

T_f : the surface tension of the fluid particle interface (MT^{-2})

ρ_f: the fluid density (ML^{-3})

g : the acceleration due to gravity [LT^{-2}]

l : the characteristic macroscopic length [L]

l_μ : the characteristic microscopic length (particle size) [L]

t: the time [T].

I am sure from this discussion; you can realize that I can write a series of parameters like this that the concentration of a contaminant in the porous media would be a function of so many properties characteristics and I hope you can guess now I am heading towards what Π-Buckingham theorem, which you have done it. So C is the concentration of contaminants in the pore water, μ is the dynamic viscosity of the fluid, D is the diffusion coefficient, S is the mass of the absorbed contaminants per unit volume.

V_s is a seepage velocity, T_f is the surface tension, ρ_f is the density of the fluid, then g the acceleration due to gravity, then L is the characteristic microscopic length and then you have time which is the physical time at which you want to find out the concentration migration and soil properties, what properties have been left out chemical characteristics, mineralogical characteristics, surface area, cation exchange capacity, its mineralogy and composition. So, once you put all these things together, this becomes a real contaminant transport through geomaterials.

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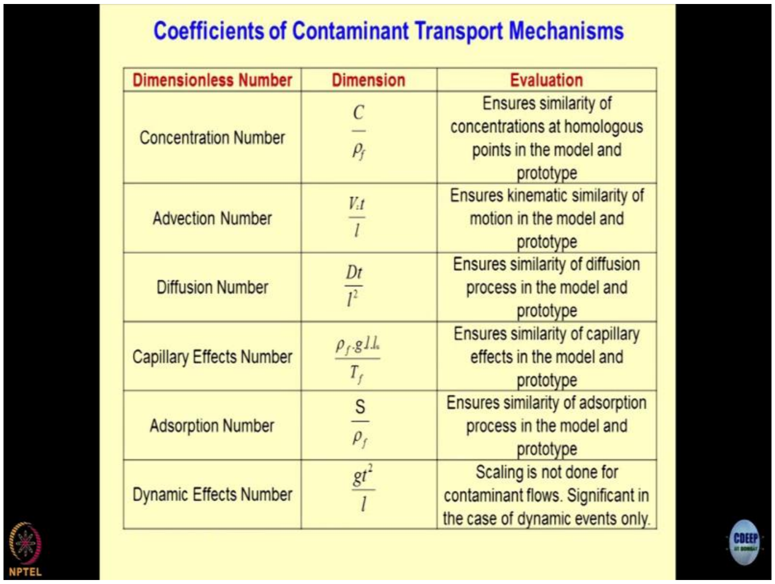

Coefficients of Contaminant Transport Mechanisms

Dimensionless Number	Dimension	Evaluation
Concentration Number	$\frac{C}{\rho_f}$	Ensures similarity of concentrations at homologous points in the model and prototype
Advection Number	$\frac{V_s t}{l}$	Ensures kinematic similarity of motion in the model and prototype
Diffusion Number	$\frac{Dt}{l^2}$	Ensures similarity of diffusion process in the model and prototype
Capillary Effects Number	$\frac{\rho_f . g\, l\, L}{T_f}$	Ensures similarity of capillary effects in the model and prototype
Adsorption Number	$\frac{S}{\rho_f}$	Ensures similarity of adsorption process in the model and prototype
Dynamic Effects Number	$\frac{gt^2}{l}$	Scaling is not done for contaminant flows. Significant in the case of dynamic events only.

Then we have different similitudes, we call them as non-dimensional numbers. So, what are the coefficients or the numbers which control the transport mechanisms, we have concentration number, addiction number, diffusion number, capillary effect number, adsorption number, dynamic effects number. So, what we have done is we could manage similitude between the numbers for some cases, and I will show you how that was done.

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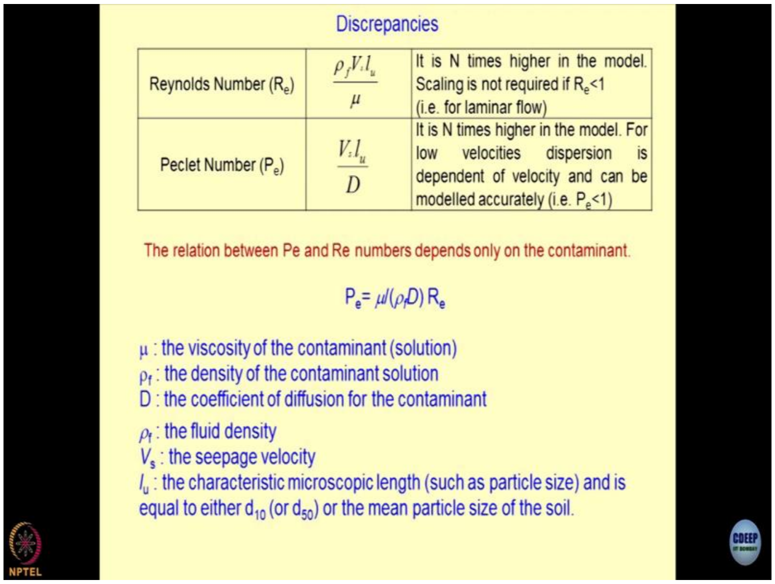

Discrepancies

Reynolds Number (R_e)	$\frac{\rho_f V_s l_u}{\mu}$	It is N times higher in the model. Scaling is not required if R_e<1 (i.e. for laminar flow)
Peclet Number (P_e)	$\frac{V_s l_u}{D}$	It is N times higher in the model. For low velocities dispersion is dependent of velocity and can be modelled accurately (i.e. P_e<1)

The relation between Pe and Re numbers depends only on the contaminant.

$$P_e = \mu/(\rho_f D)\, R_e$$

μ : the viscosity of the contaminant (solution)
ρ_f : the density of the contaminant solution
D : the coefficient of diffusion for the contaminant
ρ_f : the fluid density
V_s : the seepage velocity
l_u : the characteristic microscopic length (such as particle size) and is equal to either d_{10} (or d_{50}) or the mean particle size of the soil.

Unfortunately, there are few numbers which cannot be simulated, like the Reynolds number and Peclet numbers. So, Reynolds number I hope you understand is nothing but the initial forces divided by the viscous forces, and Peclet number talks about the diffusion coefficient, seepage velocity multiplied by the characteristic length upon the diffusion coefficient of the contaminant. Now, what I will show you is how this discrepancy was resolved.

So, if I say that the relationship between the Reynolds number and peclet number this can be proved and how this was proved, I will show you, so mu is the viscosity the contaminant in the solution form, ρ_f is the density of the contaminant, diffusion coefficient of the contaminant, density of the fluid, seepage velocity, and L_u is the microscopic length such as the particle size and normally we take it as D_{10} or D_{50}. Or the mean particle size of the soil. If you follow all this.

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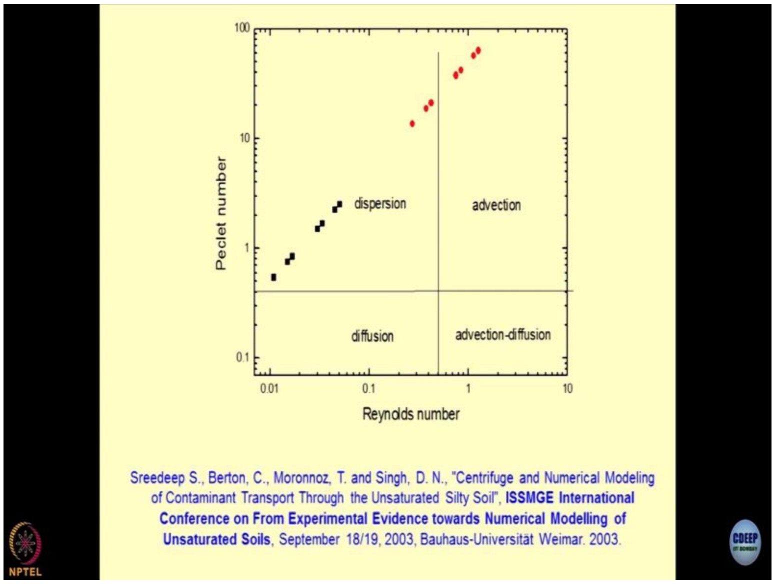

Sreedeep S., Berton, C., Moronnoz, T. and Singh, D. N., "Centrifuge and Numerical Modeling of Contaminant Transport Through the Unsaturated Silty Soil", **ISSMGE International Conference on From Experimental Evidence towards Numerical Modelling of Unsaturated Soils**, September 18/19, 2003, Bauhaus-Universität Weimar. 2003.

This is the work which some of my students did what we wanted to do is we wanted to see what type of contaminant transport occurs in compacted soils. I think this is what you are asking for some time back. So, if I plot Peclet number against the Reynolds number, this is how the situation looks like. So, I can divide the whole area of the graph into four parts, as far as the Reynolds number is less than 0.4, 0.5. And the moment it becomes >0.5.

There is a difference between the diffusive and advective diffusive contaminant transport. When the peclet number is 0.4, a combination of the Reynolds number< 0.5 and Peclet number >0.4 will create dispersion. This is proven by previous studies, Reynolds number>0.5 and peclet number >0.4 will create advection, and the fourth one is advective diffusive contaminant transport.

We did some experiments in the centrifuge and numerical modelling. And what we could show is that the type of soils normally we get, they follow advective dispersive phenomena. It was very difficult for us to create samples, where diffusive and advective diffusive contaminant transport could be created in the laboratory situation. Why? Because reconstituting the samples for a given soil where the Reynolds number, sorry, peclet number <0.4 is going to be difficult.

So, I am just trying to show you this type of study to give you a feel that simple experiments can be done to simulate a type of mechanism of contaminant transport. All these types of topics are open topics. Anybody is free to work on them and create either a porous media or a contaminant. The combination of which will give you a sort of a mechanism and you can get an answer to why this mechanism prevails.