LECTURE 37

11- APRIL - 2014

SOLUTE TRANSPORT IN POROUS MEDIA

→ Yesterday, we started the discussion on solute transport processes in porous media

→ A solute is a specie (or chemical) in dissolved or liquid state in the porous media, such that the concentration of this solute in groundwater is in dilute condition.

That is, if we consider the solute and the water as a multi-specie liquid, then the mass average density of the combined multi-specie liquid is not that much different from that of water.

→ We also discussed that some of the factors that govern the solute transport processes are:

* Advection
* Molecular diffusion
* Mechanical dispersion, etc.

→ In addition to above, there are processes like

* Chemical reactions
* Sorption
* Bio-degradation, etc.

that may also govern the solute transport processes in porous media.

Let us discuss now on each of these factors

Advection

The solute transport process due to advection is the movement of solute due to bulk movement of the liquid.
(If we recall in our earlier chapter – if we want to study the movement of one specie in a multi-specie fluid, the transport equation can be suggested of consisting of an advective component – based on mass average velocity of the multi-specie fluid – and diffusive component that is triggered due to difference between specie velocity and mass averaged velocity).

∴ In solute transport process, we consider advection due to the bulk velocity of the fluid (viz – specific discharge).

Let us consider the one-dimensional control volume as given below

Let the cross sectional area on left be $= \Delta A =$ same at right.
Only two surfaces allow flux transmission in the control volume.
→ If this CV is part of porous medium, then porous media properties like porosity, etc. to be defined.

→ Let q_x be the specific discharge in the flow direction.

→ We are now trying to infer a situation where the contaminant or solute movement is purely based on advection. (That is no other process governs the transport).

We can as usual apply RTT with mass of contaminant (or solute) in the liquid phase.

i.e. $$\frac{DB}{Dt} = 0 = \underbrace{\frac{\partial}{\partial t}\iiint \beta \rho \, dV}_{\text{Change in mass stored inside the CV}} + \underbrace{\iint_{cs} \beta \rho \, \vec{V}\cdot\hat{n} \, dA}_{\text{Net mass outflow through control surfaces}}$$

Due to advection let us define the mass flux for the contaminant as:

$$F_{a_x} = q_x C \qquad ; \quad q_x = -K\frac{\partial \phi}{\partial x}$$

(isotropic porous media)

The first integral in RHS of RTT for this case here

$$= \frac{\partial}{\partial t}\left[C\, n\, \Delta x \, \Delta A \right]$$

The second term = Net mass outflow

↳ Mass flux coming into the CV $= F_{a_x}$

↳ Mass flux going out from CV $= \left(F_{a_x} + \frac{\partial F_{a_x}}{\partial x}\Delta x \right)$

$\therefore$ Net mass outflow of contaminant from CV

$$= \left[F_{a_x} + \frac{\partial F_{a_x}}{\partial x}\Delta x\right]\Delta A - F_{a_x}\Delta A$$

$$= \frac{\partial F_{a_x}}{\partial x}\Delta x\,\Delta A = \frac{\partial}{\partial x}(q_x C)\,\Delta x\,\Delta A$$

i.e. RTT becomes

$$\frac{\partial}{\partial t}(nC)\,\Delta x\,\Delta A + \frac{\partial}{\partial x}(q_x C)\,\Delta x\,\Delta A = 0$$

or $$\boxed{\frac{\partial}{\partial t}(nC) + \frac{\partial}{\partial x}(q_x C) = 0} \rightarrow (1)$$

(1) is the advection transport equation in one-dimension

For general: $$\boxed{\frac{\partial}{\partial t}(nC) + \frac{\partial}{\partial x_i}(q_i C) = 0}$$ $i = 1, 2, 3$

If the porous medium is unsaturated with water content $= \theta$, then $\frac{\partial}{\partial t}(\theta C) + \frac{\partial}{\partial x_i}(q_i C) = 0$

Molecular diffusion

Yesterday, we discussed that molecular diffusion causes spreading of the contaminants (or solute).

$\rightarrow$ The Fick's first law:

$$F_d \propto -\frac{\partial C}{\partial x}$$

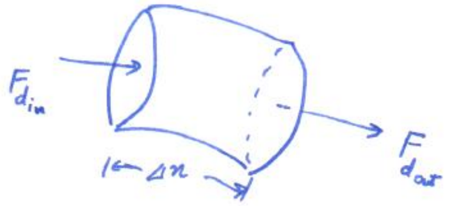
$$\text{or } F_d = -D_d \frac{\partial C}{\partial x}$$

$D_d \rightarrow$ diffusion coefft.

$\frac{\partial C}{\partial x} \rightarrow$ gradient of concn. in space.

→ The Fick's second law :

Again trying to infer solute transport process only due to molecular diffusion, consider the control volume:



Mass flux that comes in $= F_{dx}$

Mass flux that goes out $= F_{dx} + \frac{\partial F_{dx}}{\partial x} \Delta x$

Net mass of solute leaving the control volume per unit time

$$= \left(\dot{F}_{dx} + \frac{\partial F_{dx}}{\partial x} \Delta x \right) \Delta A - F_{dx} \Delta A$$

$$= \frac{\partial F_{dx}}{\partial x} \Delta x \, \Delta A$$

Change in mass storage of contaminant in the CV

$\left(\frac{\partial}{\partial t} \iiint \rho \, dV \right) \longmapsto = \frac{\partial}{\partial t} (C n) \Delta A \, \Delta x$

∴ In RTT:

$$\frac{\partial}{\partial t} (C n) \Delta A \, \Delta x \quad + \quad \frac{\partial F_{dx}}{\partial x} \Delta x \, \Delta A \quad = 0$$

i.e. $\frac{\partial}{\partial t} (n C) + \frac{\partial}{\partial x} \left(- D_d \frac{\partial C}{\partial x} \right) = 0$

or $\frac{\partial}{\partial t} (n C) = \frac{\partial}{\partial x} \left(D_d \frac{\partial C}{\partial x} \right)$

If unsaturated : $\boxed{\frac{\partial}{\partial t} (\theta C) = \frac{\partial}{\partial x} \left(D_d \frac{\partial C}{\partial x} \right)} \rightarrow$ (2)

Eq. (2) is the diffusive solute transport equation or Fick's second law.

Mechanical Dispersion

Recall when we developed the transport equations and when we did the REV averaging of parameters, we needed to incorporate a tensor D_{ij} called dispersive tensor.

⇒ When we averaged over entire REV, any flux from REV (or to REV) was suggested as composed of two parts

↳ Flux carried by average fluid motion through REV

↳ Dispersive flux resulting from velocity fluctuations.

⇒ Therefore, when we discussed about advective fluxes for solute transport, we were actually dealing with solute fluxes ~~due~~ carried by average fluid motion. Naturally there will be velocity fluctuations in the CV and we need to incorporate dispersive fluxes due to these velocity fluctuations. These are mechanical dispersions.

⇒ Dispersion actually describes the spreading of the contaminant due to velocity fluctuations. If there is no velocity, then there will be no dispersion.

* If mixing occurs in direction of flow path
  → longitudinal dispersion
* If mixing occurs in transverse direction of flow
  → transverse dispersion.

$\Rightarrow$ The phenomenon of mechanical dispersion is again explained by Fick's law.

If F_{m_x} $\rightarrow$ mass flux coming in

$F_{m_x} + \frac{\partial F_{m_x}}{\partial x} \Delta x$ $\rightarrow$ mass flux going out, etc.

Then $$\frac{\partial}{\partial t}(nc) = \frac{\partial}{\partial x}\left(D_m \frac{\partial c}{\partial x}\right)$$

However, D_m is given as

$$D_{m_L} = \alpha_L |v_L| \quad ; \text{ where } V_L = \frac{q_x}{n_e}$$

$\rightarrow$ effective porosity

$$D_{m_T} = \alpha_T |v_L|$$

where α_L and α_T are longitudinal and transverse dispersivities.

Note:- Hydrodynamic Dispersion

The process of mechanical dispersion and molecular diffusion is combinedly called hydrodynamic dispersion.

Hydrodynamic dispersion coefficient

$$\overline{D}_L = D_d + \alpha_L |v_L|$$
$$\overline{D}_T = D_d + \alpha_T |v_L|$$

To Develop Advective Dispersive Equation