LECTURE 38
17- APRIL - 2014

ADVECTIVE - DISPERSIVE EQUATION

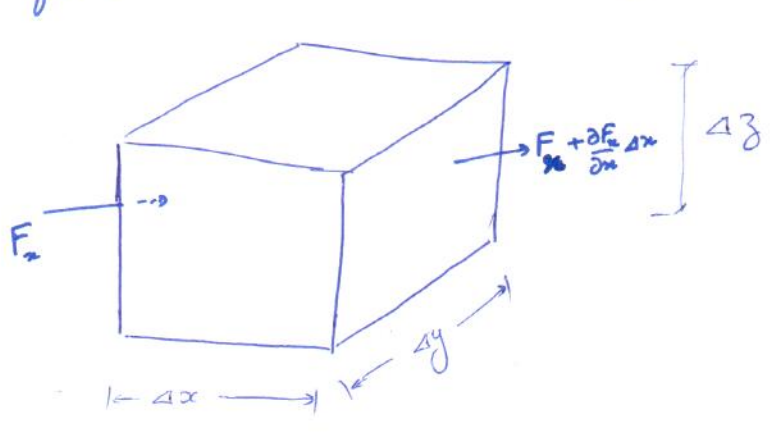
In the last class we have seen that we can associate mass transfer of solute due to

* Advection
* Molecular diffusion
* Mechanical dispersion

⇒ We have seen the fluxes associated with each of them.

⇒ We can combine all of them to arrive at the advective - dispersive transport equation

⇒ Again using the Reynolds Transport Theorem for the control volume of shape shown below:



⇒ The CV has six faces and mass can get transferred through these faces

* In the last class we independently evaluated mass transport continuity for each of the above phenomenon in one- dimension

Let advective mass flux be:

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

$$F_{a_y} = q_y c \quad ; \quad q_y = -K \frac{\partial \phi}{\partial y}$$

$$F_{a_z} = q_z c \quad ; \quad q_z = -K \frac{\partial \phi}{\partial z}$$

$\therefore$ Net mass ~~flux~~ going out from CV due to advection per unit time

$$= \frac{\partial F_{a_x}}{\partial x} \Delta x \, \Delta y \Delta z + \frac{\partial F_{a_y}}{\partial y} \Delta y \, \Delta x \Delta z + \frac{\partial F_{a_z}}{\partial z} \Delta z \, \Delta x \Delta y$$

$$= \left[\frac{\partial}{\partial x}(q_x c) + \frac{\partial}{\partial y}(q_y c) + \frac{\partial}{\partial z}(q_z c) \right] \Delta x \Delta y \Delta z$$

$\Rightarrow$ Let $\underline{\underline{D}}$ be the hydrodynamic dispersive tensor

$$D = \begin{pmatrix} D_{xx} & D_{xy} & D_{xz} \\ D_{yx} & D_{yy} & D_{yz} \\ D_{zx} & D_{zy} & D_{zz} \end{pmatrix}$$

This includes both the molecular diffusion and mechanical dispersion combined coefficient.

If the ~~directions~~ axes are ϕ in principal directions,

$$\underline{\underline{D}} = \begin{pmatrix} D_{xx} & 0 & 0 \\ 0 & D_{yy} & 0 \\ 0 & 0 & D_{zz} \end{pmatrix}$$

③

∴ The net mass outflow of solute from the CV per unit time due to dispersion

$$= \frac{\partial F_{dx}}{\partial x} \Delta x \Delta y \Delta z . n + \frac{\partial F_{dy}}{\partial y} \Delta y \Delta x \Delta z . n$$

$$+ \frac{\partial F_{dz}}{\partial z} \Delta z \Delta x \Delta y . n$$

{Assuming the porous media is saturated}

$$= \left(\frac{\partial F_{dx}}{\partial x} + \frac{\partial F_{dy}}{\partial y} + \frac{\partial F_{dz}}{\partial z} \right) n \Delta x \Delta y \Delta z$$

where

$$F_{dx} = - D_{xx} \frac{\partial C}{\partial x}$$

$$F_{dy} = - D_{yy} \frac{\partial C}{\partial y}$$

$$F_{dz} = - D_{zz} \frac{\partial C}{\partial z}$$

∴ Net mass of outflow of solute due to hydrodynamic dispersion per unit time

$$= \left(-\frac{\partial}{\partial x}\left(D_{xx} \frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial y}\left(D_{yy} \frac{\partial C}{\partial y}\right) - \frac{\partial}{\partial z}\left(D_{zz} \frac{\partial C}{\partial z}\right) \right) n \Delta x \Delta y \Delta z$$

∴ Net mass outflow per unit time due to advection & hydrodynamic dispersion :

$$= \left[\frac{\partial}{\partial x}(q_x C) + \frac{\partial}{\partial y}(q_y C) + \frac{\partial}{\partial z}(q_z C) - \frac{\partial}{\partial x}\left(D_{xx} \frac{\partial C}{\partial x}\right) n - \frac{\partial}{\partial y}\left(D_{yy} \frac{\partial C}{\partial y}\right) n - \frac{\partial}{\partial z}\left(D_{zz} \frac{\partial C}{\partial z}\right) n \right] \Delta x \Delta y \Delta z$$

The first term of RTT in the RHS

i.e. $\frac{\partial}{\partial t}\iiint_{cv} \beta \rho \, dV$ for this case

$$= \frac{\partial}{\partial t}(nc)\, \Delta x \Delta y \Delta z$$

$\Rightarrow$ RTT $\left[\frac{\partial}{\partial t}\iiint_{cv} \beta \rho \, dV + \iint_{cs} \beta \rho \, \vec{V}\cdot\hat{n}\, dA = 0 \right]$

becomes

$$\frac{\partial}{\partial t}(nc)\, \Delta x \Delta y \Delta z + \left[\frac{\partial}{\partial x}(q_x c) + \frac{\partial}{\partial y}(q_y c) + \frac{\partial}{\partial z}(q_z c) - \frac{\partial}{\partial x}\left(D_{xx} n \frac{\partial c}{\partial x}\right) - \frac{\partial}{\partial y}\left(D_{yy} n \frac{\partial c}{\partial y}\right) - \frac{\partial}{\partial z}\left(D_{zz} n \frac{\partial c}{\partial z}\right)\right] \Delta x \Delta y \Delta z = 0$$

Considering $\Delta x \Delta y \Delta z$ as fixed; we get the Advective - Dispersive Equation:

$$\boxed{\frac{\partial}{\partial t}(nc) + \frac{\partial}{\partial x}(q_x c) + \frac{\partial}{\partial y}(q_y c) + \frac{\partial}{\partial z}(q_z c) = \frac{\partial}{\partial x}\left(D_{xx} n \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial y}\left(D_{yy} n \frac{\partial c}{\partial y}\right) + \frac{\partial}{\partial z}\left(D_{zz} n \frac{\partial c}{\partial z}\right)}$$

In index notation.

$$\boxed{\frac{\partial (nc)}{\partial t} + \frac{\partial}{\partial x_i}(q_i c) = \frac{\partial}{\partial x_i}\left(D_{ij}\, n \frac{\partial c}{\partial x_j}\right)}$$

In the saturated porous medium, if $\frac{q_x}{n} = v_x$ (seepage velocity component in x-direction).

$\frac{q_y}{n} = v_y$; $\frac{q_z}{n} = v_z$

Also assuming $\frac{\partial n}{\partial t} \approx 0$, so well as $\frac{\partial n}{\partial x_i} = 0$,

we get ADE as:

$$\boxed{\frac{\partial}{\partial t} c + \frac{\partial}{\partial x_i}(v_i c) = \frac{\partial}{\partial x_i}\left(D_{ij} \frac{\partial c}{\partial x_j}\right)}$$

Advective - Dispersive Transport with Retardation

In the previous portion we discussed about advection and dispersion.

⇒ If the solute (or contaminant) interacts with the solid grains inside the CV of the porous media, then the ADE needs to incorporate terms for this interaction

⇒ One particular process is Sorption

* It is the physical or chemical process through which the solute attach with the solid grains
* If the solute from liquid attach to the solid, then naturally the movement of this solute through liquid in porous

media gets retarded.

* The mechanism can subsequently be explained through retarded solute transport equation.

If c is the concentration of solute in liquid (ML^{-3})
v_x is the average linear velocity of groundwater in x-direction, $\rho_b \rightarrow$ bulk density of the porous medium or aquifer

$n \rightarrow$ porosity of the medium

$S \rightarrow$ amount of solute sorbed into the solids per unit weight of the solid

Then mathematically we need to modify ADE as:

$$\frac{\partial}{\partial t}(nc) + \frac{\partial}{\partial x}(q_x c) - \frac{\partial}{\partial x}\left(n D_{xx} \frac{\partial c}{\partial x}\right) + R_s = 0 \quad \rightarrow (1)$$

where $R_s \rightarrow$ the term corresponding for sorption that causes change in mass of solute.

We can determine them through RTT itself

→ Sorption is not something that causes flux through control surfaces.

Therefore only the portion $\frac{\partial}{\partial t}\iiint_{cv} \beta \, g \, dV$ in the RTT will change due to sorption

In the control volume $\Delta x \, \Delta y \, \Delta z$:

$\Rightarrow$ The change in mass of solute per unit time due to sorption :

$$= \frac{\partial}{\partial t}\left(\rho_b \, S\right) \Delta x \, \Delta y \, \Delta z$$

$\therefore$ R_s in eqn. 1 will be $\frac{\partial}{\partial t}(\rho_b \, S)$ and it will decrease mass of solute in liquid phase.

i.e.

$$\frac{\partial}{\partial t}(nc) + \frac{\partial}{\partial x}(q_x \, c) - \frac{\partial}{\partial x}\left(n \, D_{xx} \frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial t}(\rho_b \, S) = 0$$

Actually we should infer this as:

$$\left[\frac{\partial}{\partial t}\iiint_{cv} \beta \, g \, dV = \left[\frac{\partial}{\partial t}(nc) + \rho_b \frac{\partial S}{\partial t}\right] \Delta x \, \Delta y \, \Delta z\right]$$

$\therefore$ Our ADE becomes

$$\frac{\partial}{\partial t}(nc) + \rho_b \frac{\partial S}{\partial t} + \frac{\partial}{\partial x}(q_x \, c) = \frac{\partial}{\partial x}\left(n \, D_{xx} \frac{\partial c}{\partial x}\right)$$

If the porous media is isotropic and homogeneous (of course saturated), then

$$\frac{\partial c}{\partial t} + \frac{\rho_b}{n} \frac{\partial S}{\partial t} + \frac{\partial}{\partial x}(V_x \, c) = \frac{\partial}{\partial x}\left(D_{xx} \frac{\partial c}{\partial x}\right)$$

$\hookrightarrow$ 2

The sorption can be explained through various sorption isotherms:

1) Linear Sorption Isotherm:

$$S = K_d\, C \quad \rightarrow (3)$$

where $K_d \rightarrow$ distribution coefficient

Then Substituting (3) in (2),

$$\frac{\partial C}{\partial t} + \frac{\rho_b}{n}\frac{\partial}{\partial t}(K_d C) + \frac{\partial}{\partial x}(V_x C) = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x}\right)$$

i.e.
$$\left(1 + \frac{\rho_b}{n}K_d\right)\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial x}(V_x C)$$

as defining retardation factor $R = 1 + \frac{\rho_b}{n}K_d$

we get:

$$\boxed{R\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(D_{xx}\frac{\partial C}{\partial x}\right) - \frac{\partial}{\partial x}(V_x C)}$$

Retarding solute transport phenomenon using linear isotherms.