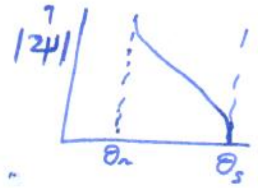
LECTURE 36
10-APR-2014

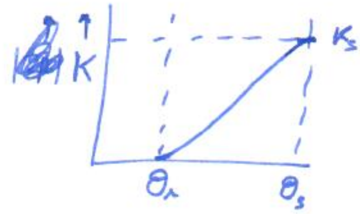
SOLUTE TRANSPORT

In the last class we were dealing with unsaturated flow.

* We have seen that the moisture content and suction head are related that can be expressed by empirical relations described by many scientists — viz: Gardner (1958), Brooks and Corey (1964), van Genuchten (1980), etc.



* In a similar tone we can also related hydraulic conductivity with water content and subsequently with suction head.



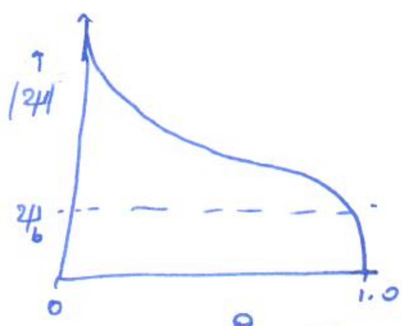
* The one dimensional Richards equation

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z}\left(D \frac{\partial \theta}{\partial z} + K \right)$$

can be solved using these constitutional relationships.

For example

1) The Brooks-Corey relationship between moisture content and suction head is

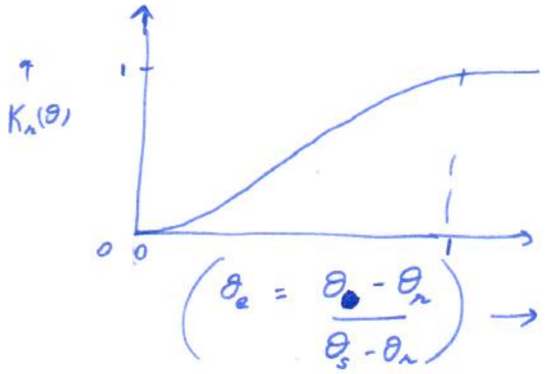


$$\theta_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left(\frac{\psi_b}{\psi}\right)^{\lambda}$$

Brooks and Corey (1964) have also given relationships between K and θ.

$$\frac{K(\theta)}{K_s} = K_r(\theta) = (\theta_e)^n$$

where $n = 3 + \frac{2}{\lambda}$



2) Similarly van-Genuchten have given relationships between θ and ψ as such:

$$\theta_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \left[\frac{1}{1 + (\alpha|\psi|)^n}\right]^m$$

where $\alpha \rightarrow$ parameter related to air entry pressure $[L^{-1}]$
$n \rightarrow$ constant
$m \rightarrow$ constant

$K_r(\theta) =$

SOLUTE TRANSPORT

In groundwater hydrology, we have seen about flow in aquifers, well hydraulics, briefly about unsaturated ~~ka~~ zone hydrology, etc.

* An important subject for a groundwater hydrologist is Contaminant transport modeling.

⇒ The groundwater ~~sources~~ bodies are highly vulnerable to contamination from various sources like:

* Septic tanks, Oil disposals, landfill leaching, mine wastes and drainages, tannery, pesticides, etc.

⇒ We know that the speed of groundwater is very slow compared to surface water bodies. Therefore, if any contaminant enters into a groundwater system, it may remain there for a long time. So it may not be possible to wash away the contaminants at rapid speed.

⇒ Scientific studies of contaminant movement through subsurface — including aquifers and unsaturated zones are essential to understand the impacts and extents of contamination at any region.

Recalling our earlier chapters - ~~e~~ viz: Chapter 4 where we dealt with continuity and momentum equations for multi-specie fluid, we can employ same principles here.

i.e. ~~Convection~~

⇒ A porous medium subjected to a certain contamination may be considered as a multi-specie fluid.

∴ Based on mass-averaged velocity $\vec{V}^*$, you can have diffusive and dispersive components for ~~contaminants~~ the respective contaminant species.

⇒ Modelling such contaminant transport are essential for groundwater contamination mitigation

⇒ The processes that involve contaminant transport are :
→ Advection
→ Diffusion
→ Dispersion

In contaminant transport studies : the

Molecular diffusion

The solute or contaminant moves from higher concentration to lower concentration and is called diffusion.

The term concentration suggest about the strength or portion of contaminant in the water. The units may be $\rightarrow$ ~~m~~ $\dfrac{\text{mass of contaminant}}{\text{Unit volume of water}}$

or ~~p~~ mass of contaminant per unit mass of water, etc.

$\Rightarrow$ The term diffusion suggest about ~~diffusion~~ spreading of the contaminants.

Contaminant initially concentrated at a location

After some time the contaminant intensity decreased but spread more in the domain

$\Rightarrow$ The laws of diffusion are very much applicable to the situation here:

Fick's first law:

If 'F' is mass flux of solute (~~per~~ or contaminant) per unit time per unit area (i.e. $ML^{-2}T^{-1}$ like $\frac{kg}{m^2 s}$ etc.)

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

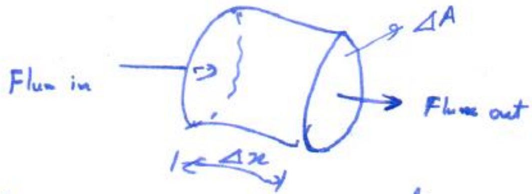
$$F = -D_d \frac{\partial C}{\partial x}$$

(See the analogy w.r.t. Darcy's law)

where $D_d \rightarrow$ diffusion coefficient

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

Ficks second law :



Considering a one dimensional control volume shown above, let the mass come into CV from left and goes out through right

Let mass flux that comes in $= F$

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

Mass entering the control volume per unit time $= F \, \Delta A$

Mass leaving control volume per unit time $= \left(F + \frac{\partial F}{\partial x} \Delta x\right) \Delta A$

$\therefore$ ~~Net mass~~ Using Reynolds Transport theorem for mass conservation of solute

$$0 = \frac{\partial}{\partial t} \iiint \beta \rho \, dU + \iint_{\omega} \beta \rho (\vec{V} \cdot \hat{n}) \, dA$$

$\iint_{\omega} \rho (\vec{V} \cdot \hat{n}) \, dA \rightarrow$ Net mass outflow per unit time

$$= \frac{\partial F}{\partial x} \Delta x \, \Delta A$$

(for the case of diffusion here)

$\frac{\partial}{\partial t} \iiint \rho \, dU \rightarrow$ Change in mass ~~stored~~ of contaminant stored in CV.

$$= \frac{\partial}{\partial t} (C \, \Delta A \, \Delta x)$$

$$\therefore \quad \frac{\partial C}{\partial t} \Delta x \, \Delta A = - \frac{\partial F}{\partial x} \Delta x \, \Delta A$$

or $$\frac{\partial c}{\partial t} = -\frac{\partial F}{\partial x}$$

Recall $$F = -D_d \frac{\partial c}{\partial x}$$

$$\therefore \frac{\partial c}{\partial t} = -\frac{\partial}{\partial x}\left(-D_d \frac{\partial c}{\partial x}\right)$$

$$\text{ie} \quad \frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D_d \frac{\partial c}{\partial x}\right)$$

If diffusivity D_d is independant of space,

$$\frac{\partial c}{\partial t} = D_d \frac{\partial^2 c}{\partial x^2}$$ (Fick's second law :)

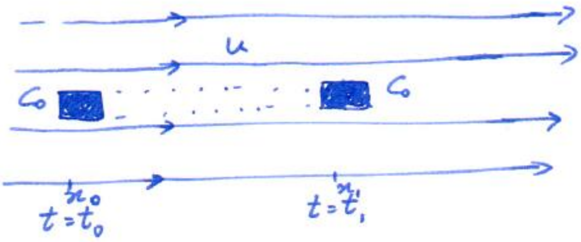
Mechanical Dispersion

The contaminant transport in addition to molecular diffusion may occur due to mechanical dispersion.
→ As the term suggests this is caused by mechanical process. Mixing of contaminant occurs due to difference in speeds of movement of contaminants

Before discussing mechanical dispersion, we should discuss first about contaminant transport process through advection.

The mass movement due to bulk motion of fluid describes the advection.

i.e. In a uniform flow field



In the figure/the description given here, the contaminant with concentration C_0 is applied at $x = x_0$ in uniform flow field.

If the concentration of the contaminant is C_0 at time $t = t_1$ at $x = x_1$ with same dimension, this means that the contaminant has not spread and the movement of contaminant occurred purely due to the bulk movement of water.

=> If there is difference in such bulk velocities or advective velocities, then a gradient exist that can cause dispersive contaminant mass flux.

$$F_m = -D_m \frac{\partial C}{\partial x} \quad \text{and} \quad \left.\frac{\partial C}{\partial t}\right|_m = \frac{\partial}{\partial x}\left(-D_m \frac{\partial C}{\partial x}\right)$$

where $D_m = \alpha_L V_L$

$\alpha_L \rightarrow$ longitudinal mechanical dispersivity

$V_L \rightarrow$ pore velocity