Contaminant Transport Equations

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Transport

Advection

- The process by which solutes are transported by the bulk of motion of the flowing ground water.
- Nonreactive solutes are carried at an average rate equal to the average linear velocity of the water.

Hydrodynamic Dispersion

- Tendency of the solute to spread out from the advective pathway
- Two processes

    Diffusion (molecular and turbulent)

    Dispersion (velocity differences in space)

Diffusion

- Ions (molecular constituents) in solution move under the influence of kinetic activity in direction of their concentration gradients.
- Occurs in the absence of any bulk hydraulic movement
- Diffusive flux is proportional to concentration gradient, per *Fick's First Law ($M\ L^{-2}T^{-1}$).*

$$F = -D_m\left(\frac{dc}{dx}\right)$$

- Where D_m = diffusion coefficient (typically 1 x 10^{-5} to 2 x 10^{-5} $cm^{2/}s$ for major ions in ground water)

Diffusion (continued)

- ***Fick's Second Law*** - derived from Fick's First Law and the Continuity Equation - called "Diffusion Equation"

$$\frac{\partial C}{\partial t} = D_m \left(\frac{\partial^2 C}{\partial x^2} \right)$$

The Advection-Dispersion Equation Derivation (F is transport flux)

Assumptions:

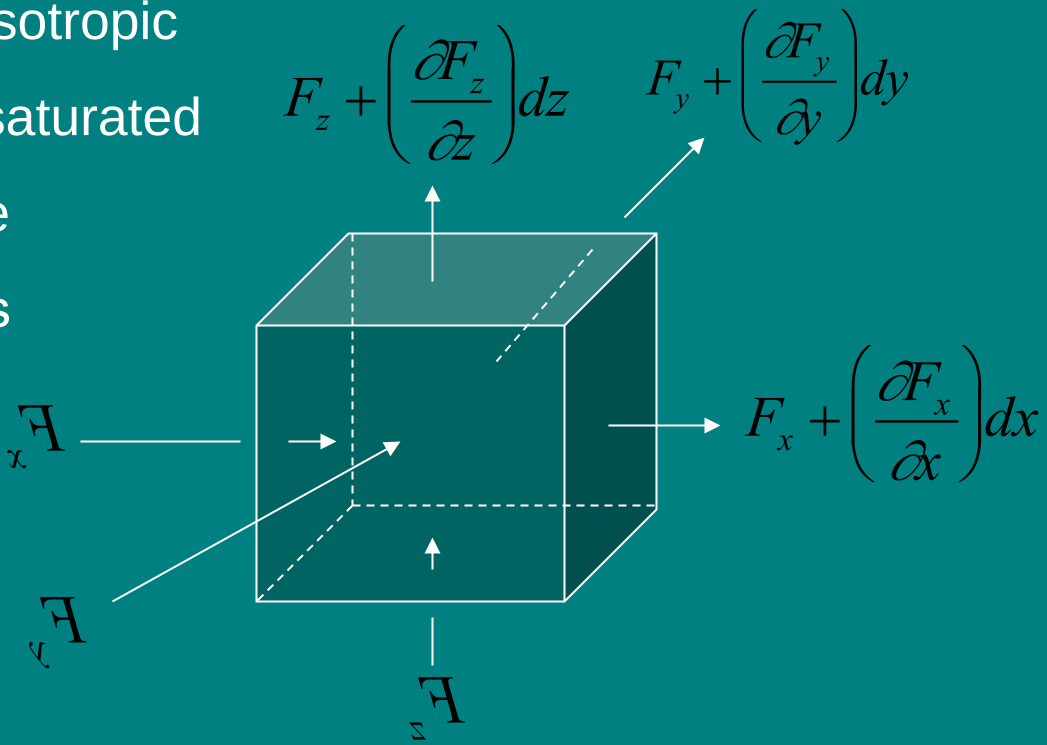
1) Porous medium is homogenous

2) Porous medium is isotropic

3) Porous medium is saturated

4) Flow is steady-state

5) Darcy’s Law applies



Advection Dispersion Equation

In the x-direction:

Transport by advection = $\bar{v}_x nCdA$ units $\frac{M}{T}$

Transport by dispersion = $nD_x\left(\frac{\partial C}{\partial x}\right)dA$ $units\ \frac{M}{T}$

Where:

$\bar{v}$ = average linear velocity

n = porosity (constant for unit of volume)

C = concentration of solute

dA = elemental cross-sectional area of cubic element

$$D_x = \alpha_x \bar{v}_x + D_m$$

Hydrodynamic Dispersion D_x caused by molecular diffusion and variations in the velocity field and heterogeneities

where:

α_x = dispersivity [L]

D_m = Molecular diffusion

$$F_x = v_x nC - nD_x \left(\frac{\partial C}{\partial x} \right)$$

- Flux = (mass/area/time)

(-) sign before dispersion term indicates that the contaminant moves toward lower concentrations

$$F_x = v_x nC - nD_x \left(\frac{\partial C}{\partial x} \right)$$

- Total amount of solute entering the cubic element

$$= F_x dydz + F_y dxdz + F_z dxdy$$

- Difference in amount entering and leaving element =

$$\left(\frac{\partial F_x}{\partial x} + \frac{\partial F_y}{\partial y} + \frac{\partial F_z}{\partial z}\right) dxdydz$$

- For nonreactive solute, difference between flux in and out = amount accumulated within element

- Rate of mass change in element =

$$n\left(\frac{\partial C}{\partial t}\right) dxdydz$$

- Equate two equations and divide by $dV = dxdydz$:

$$-\left(\frac{\partial F_x}{\partial x}\right)+\left(\frac{\partial F_y}{\partial y}\right)+\left(\frac{\partial F_z}{\partial z}\right)=n\left(\frac{\partial C}{\partial t}\right)$$

- Substitute for fluxes and cancel n:

$$-\left[\frac{\partial}{\partial x}\left(\bar{v}_x C\right)+\frac{\partial}{\partial y}\left(\bar{v}_y C\right)+\frac{\partial}{\partial z}\left(\bar{v}_z C\right)\right]+$$

$$\left\{\frac{\partial}{\partial x}\left[D_x\left(\frac{\partial C}{\partial x}\right)\right]+\frac{\partial}{\partial y}\left[D_y\left(\frac{\partial C}{\partial y}\right)\right]+\frac{\partial}{\partial z}\left[D_z\left(\frac{\partial C}{\partial z}\right)\right]\right\}=\frac{\partial C}{\partial t}$$

- For a homogenous and isotropic medium, $\bar{v}$ is steady and uniform.

- For a homogenous and isotropic medium,   is steady and uniform.
- Therefore, D_x, D_y, *and* D_z do not vary through space.

$$\left[D_x\left(\frac{\partial^2 C}{\partial x^2}\right)+D_y\left(\frac{\partial^2 C}{\partial y^2}\right)+Dz\left(\frac{\partial^2 C}{\partial z^2}\right)\right]$$

- **Advection-Dispersion Equation 3-D:**

$$-\left[\bar{v}_x\left(\frac{\partial C}{\partial x}\right)+\bar{v}_y\left(\frac{\partial C}{\partial y}\right)+\bar{v}_z\left(\frac{\partial C}{\partial z}\right)\right]=\frac{\partial C}{\partial t}$$

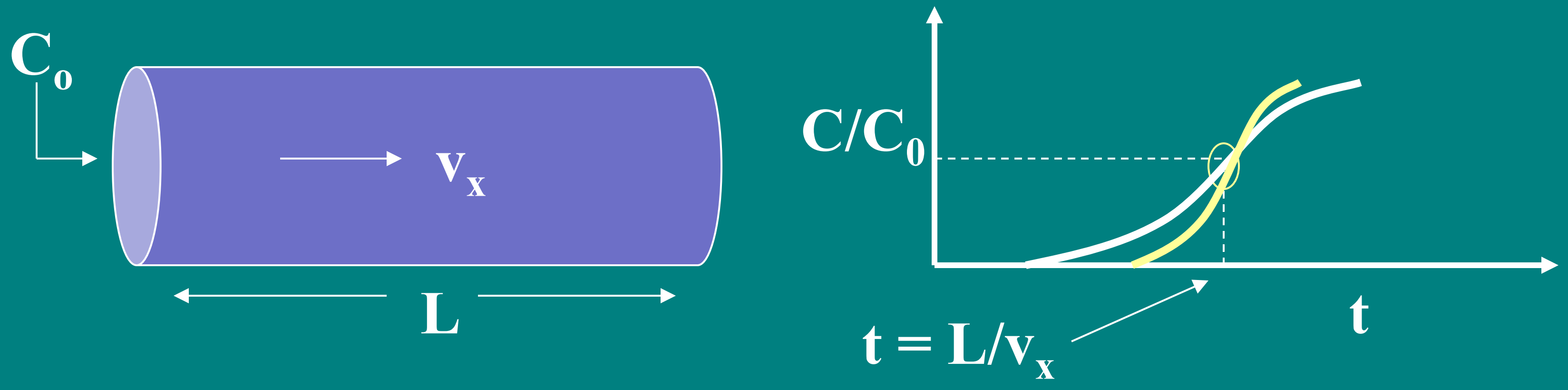
In 1-D, the AD equation thus becomes:

$$\frac{\partial C}{\partial t} + \bar{v}_x \left(\frac{\partial C}{\partial x} \right) = D_x \left(\frac{\partial^2 C}{\partial x^2} \right)$$

Accumulation **Advection** **Dispersion**

CONTINUOUS SOURCE

- Solution for 1-D Equation for can be found using Laplace Transform



- 1-D soil column breakthrough curves

Solution can be written **(Ogato & Banks, 1961)**

$$\frac{C}{C_0} = \frac{1}{2} Erfc\left(\frac{L - v_x t}{\sqrt{4 D_x t}}\right) + \left(\frac{1}{2}\right) Exp\left(\frac{v_x L}{D_x}\right) Erfc\left(\frac{L - v_x t}{\sqrt{4 D_x t}}\right)$$

or, in most cases

$$\frac{C}{C_0} = \frac{1}{2} Erfc\left(\frac{L - v_x t}{\sqrt{4 D_x t}}\right)$$

where

$$Erfc(B) = 1 - Erf(B)$$

$$Erf(B) = \frac{2}{\sqrt{\pi}} \int_0^B e^{-z^2} dz$$

Tabulated error function

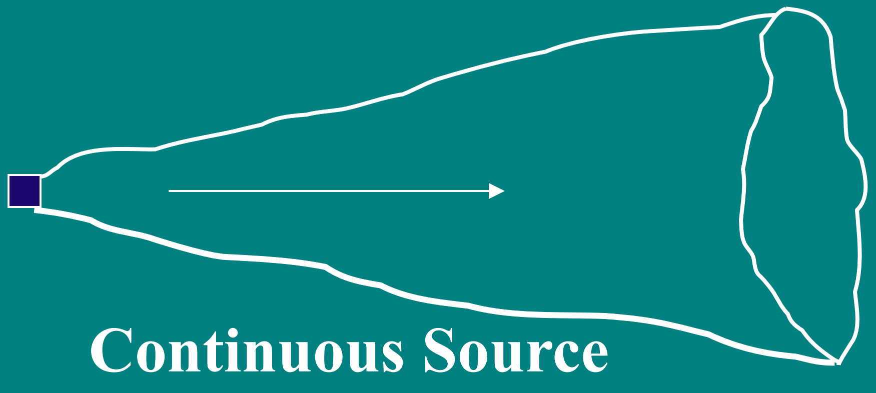
Instantaneous Sources
Advection-Dispersion Only

Instantaneous POINT Source 3-D:

$$C(x,y,z,t) = \frac{M}{(4\pi Dt)^{3/2}} \exp\left(-\frac{(x-vt)^2}{4D_x t} - \frac{y^2}{4D_y t} - \frac{z^2}{4D_z t} \right)$$

$M = C_0 V$

$D = (D_x D_y D_z)^{1/3}$



Instantaneous LINE Source 2-D Well:

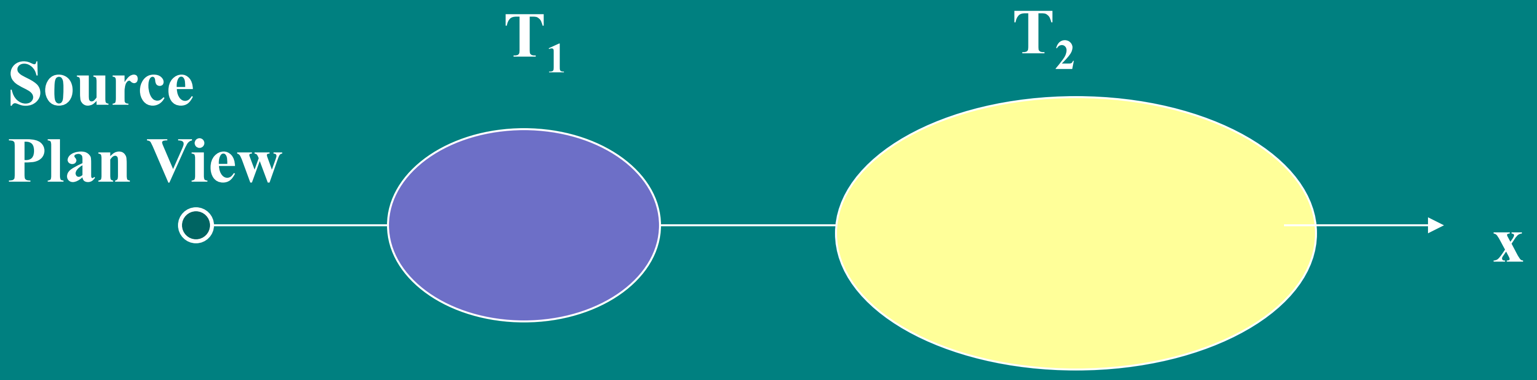
(with First Order Decay)

$$C(x,y,t) = \frac{m}{4\pi D t} \exp\left(-\frac{(x - vt)^2}{4 D_x t} - \frac{y^2}{4 D_y t} - kt \right)$$

$k =$ *first order decay* (t^{-1})

$m = C_o A$

$D = \sqrt{D_x D_y}$



Instantaneous PLANE Source - 1 D

$$C(x,t) = \frac{M}{\sqrt{4\pi D_x t}}\, Exp\left(-\frac{(x - vt)^2}{4D_x t}\right)$$

$$M = \frac{mass}{area}$$

AD Equation

$$\frac{\partial C}{\partial t} + \bar{v}_x \left(\frac{\partial C}{\partial x}\right) = D_x \left(\frac{\partial^2 C}{\partial x^2}\right)$$