

HWRS 561b: Physical Hydrogeology II

Solute transport (Part 2)

Agenda:

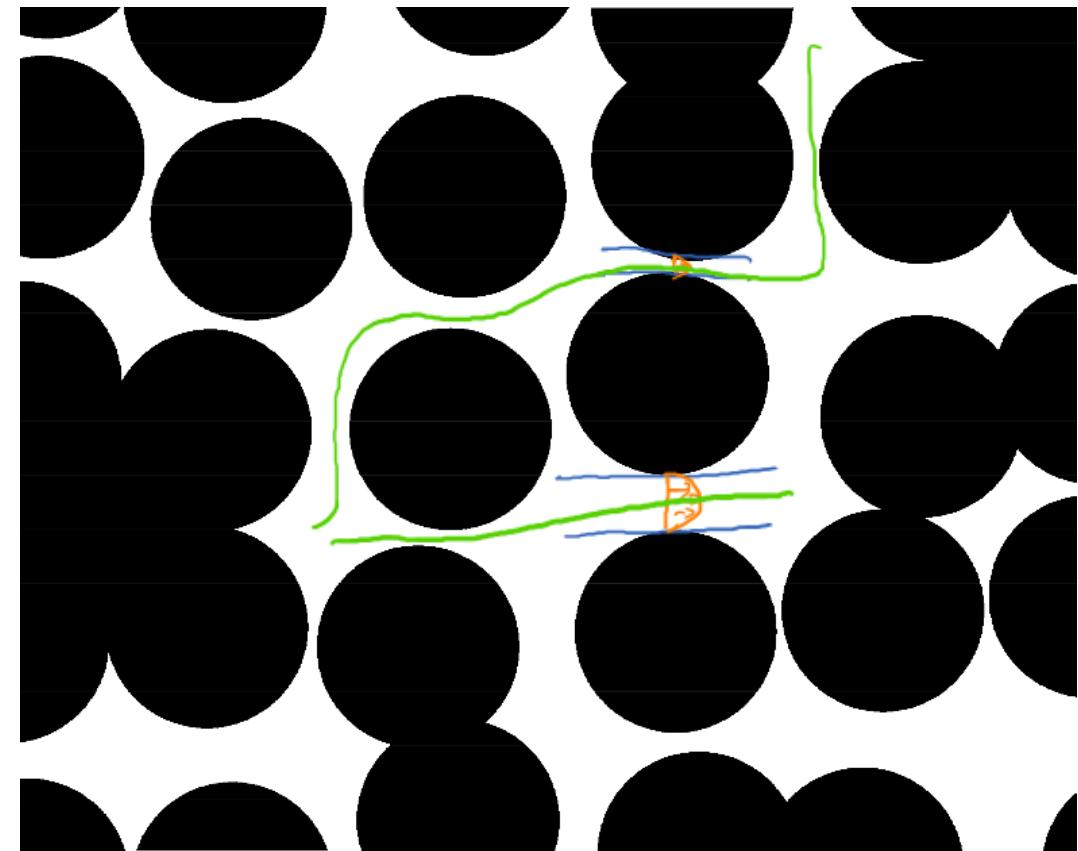
1. Basic concepts
2. Flux law
3. Derivation of solute transport equation

Solute transport under saturated flow

Taylor-Aris Dispersion: Spatial variation of velocity leads to dispersion of solutes

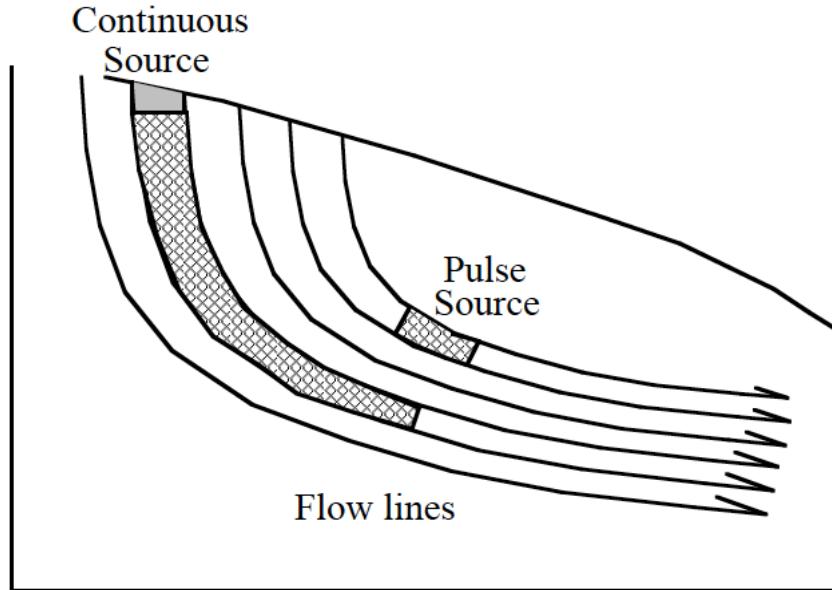
Spatial variation of velocity in a porous medium:

- (1) Velocity profile through a pore throat (related to T-A dispersion)
- (2) Velocity variation among pore throats
- (3) Tortuosity

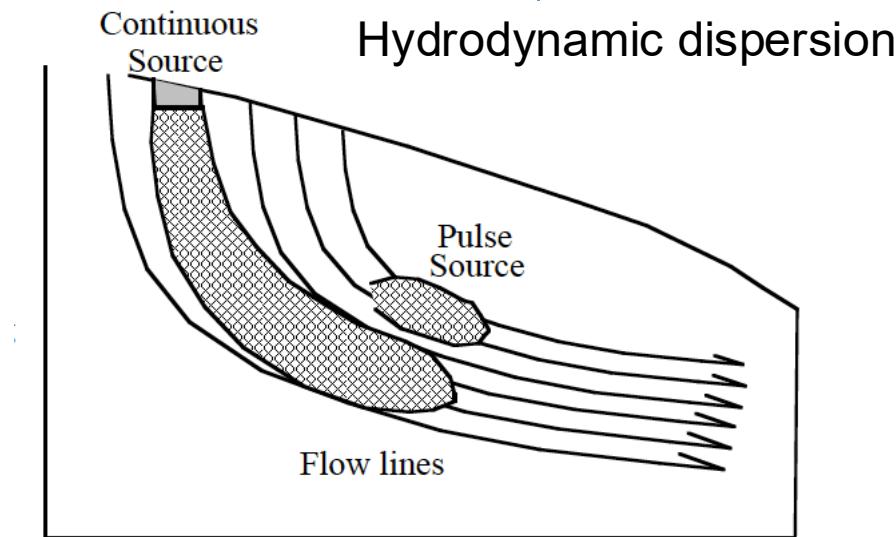


Solute transport under saturated flow

Pure advection

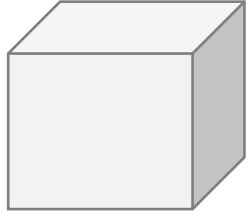


Advection + Mechanical dispersion + Molecular diffusion

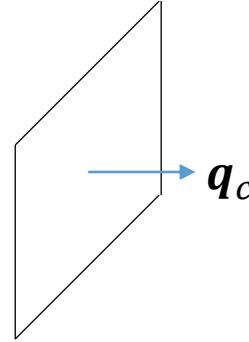


Solute transport under saturated flow

A widely used theory for describing solute flux in saturated porous media [J. Bear (1961)]

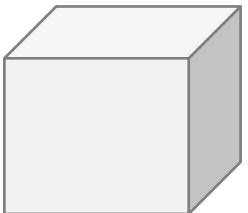


Saturated
porous medium

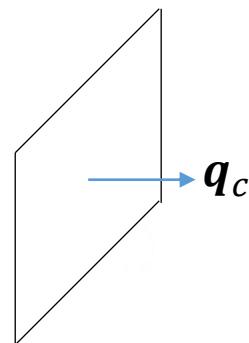


$$\mathbf{q}_c = \phi(\mathbf{v}C - \mathbf{D}\nabla C),$$

- \mathbf{q}_c is the solute flux vector.
- \mathbf{v} is the velocity field.
- \mathbf{D} is a tensor that depends on the velocity field and molecular diffusion in the porous medium.



Fluid only
(e.g., free water)



$$\mathbf{q}_c = \mathbf{v}C - D_0\nabla C$$

Diffusion is isotropic,
not a tensor.

Solute transport under saturated flow

$$\begin{aligned} \mathbf{q}_c &= \phi(\mathbf{v}\mathbf{C} - \mathbf{D}\nabla\mathbf{C}) \\ &= \mathbf{q}\mathbf{C} - \phi\mathbf{D}\nabla\mathbf{C} \end{aligned}$$

For a special case in 1D flow (v_y and v_z are zero)

$$D_{xx} = \alpha_L v_x + D_d$$

$$D_{yy} = D_{zz} = \alpha_T v_x + D_d$$

$$\mathbf{D} = \begin{pmatrix} \alpha_L |\mathbf{v}| + wD_0 & 0 & 0 \\ 0 & \alpha_T |\mathbf{v}| + wD_0 & 0 \\ 0 & 0 & \alpha_T |\mathbf{v}| + wD_0 \end{pmatrix}$$

Outer product $\underline{\mathbf{v}}\underline{\mathbf{v}} \cdot \underline{\mathbf{x}} = \underline{\mathbf{x}}(\underline{\mathbf{v}} \cdot \underline{\mathbf{x}})$

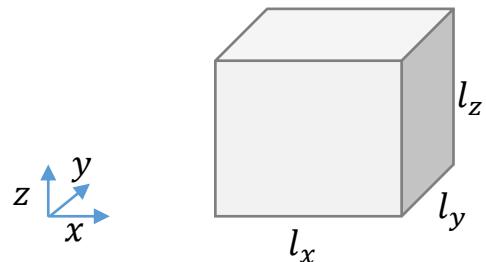
$$\mathbf{D} = \alpha_T |\mathbf{v}| \mathbf{I} + (\alpha_L - \alpha_T) \frac{\mathbf{v}\mathbf{v}}{|\mathbf{v}|} + wD_0 \mathbf{I} \quad \alpha_L \text{ and } \alpha_T \text{ are longitudinal and transverse dispersivities, respectively.}$$

$$\mathbf{D} = \begin{pmatrix} \alpha_T |\mathbf{v}| + wD_0 + \frac{\alpha_L - \alpha_T}{|\mathbf{v}|} v_x^2 & \frac{\alpha_L - \alpha_T}{|\mathbf{v}|} v_x v_y & \frac{\alpha_L - \alpha_T}{|\mathbf{v}|} v_x v_z \\ \frac{\alpha_L - \alpha_T}{|\mathbf{v}|} v_y v_x & \alpha_T |\mathbf{v}| + wD_0 + \frac{\alpha_L - \alpha_T}{|\mathbf{v}|} v_y^2 & \frac{\alpha_L - \alpha_T}{|\mathbf{v}|} v_y v_z \\ \frac{\alpha_L - \alpha_T}{|\mathbf{v}|} v_z v_x & \frac{\alpha_L - \alpha_T}{|\mathbf{v}|} v_z v_y & \alpha_T |\mathbf{v}| + wD_0 + \frac{\alpha_L - \alpha_T}{|\mathbf{v}|} v_z^2 \end{pmatrix}$$

$$q_{c,x} = \left[\alpha_T |\mathbf{v}| + (\alpha_L - \alpha_T) \frac{v_x^2}{|\mathbf{v}|} + wD_0 \right] \frac{\partial C}{\partial x} + \left[(\alpha_L - \alpha_T) \frac{v_x v_y}{|\mathbf{v}|} \right] \frac{\partial C}{\partial y} + \left[(\alpha_L - \alpha_T) \frac{v_x v_z}{|\mathbf{v}|} \right] \frac{\partial C}{\partial z}$$

q_y and q_z can be written out in a similar way.

Solute transport under saturated flow



$$C(x, y, z, t) = \frac{\text{mass of solute}}{\text{unit fluid volume}}$$

Mass conservation: Change of mass storage = mass in – mass out.

Rate of mass change: $\frac{\partial}{\partial t} \int_0^{l_x} \int_0^{l_y} \int_0^{l_z} \phi(x, y, z, t) C(x, y, z, t) dx dy dz = \frac{\partial}{\partial t} \int_{\Omega} \phi C dv$

Net fluxes:

$$-\int_{\Omega} q \cdot n dv = -\int_{\Omega} q_c \cdot n ds \left\{ \begin{array}{l} + \int_0^{l_x} \int_0^{l_y} q_{c,x} \Big|_{x=0} - \int_0^{l_y} \int_0^{l_z} q_{c,x} \Big|_{x=l_x} \\ + \int_0^{l_x} \int_0^{l_z} q_{c,y} \Big|_{y=0} - \int_0^{l_x} \int_0^{l_z} q_{c,y} \Big|_{y=l_y} \\ + \int_0^{l_y} \int_0^{l_z} q_{c,z} \Big|_{z=0} - \int_0^{l_x} \int_0^{l_y} q_{c,z} \Big|_{z=l_z} \end{array} \right.$$

Solute transport under saturated flow

$$\frac{\partial}{\partial t} \int_{\Omega} \phi c \, dv = - \int_{\Omega} \nabla \cdot \underline{q}_c \, dv$$

$\downarrow \Omega \neq \Omega(t)$

$$\Rightarrow \int_{\Omega} \frac{\partial}{\partial t} (\phi c) \, dv = - \int_{\Omega} \nabla \cdot \underline{q}_c \, dv$$

$$\Rightarrow \int_{\Omega} \left[\frac{\partial}{\partial t} (\phi c) + \nabla \cdot \underline{q}_c \right] \, dv = 0$$

$\downarrow \Omega$ is arbitrary

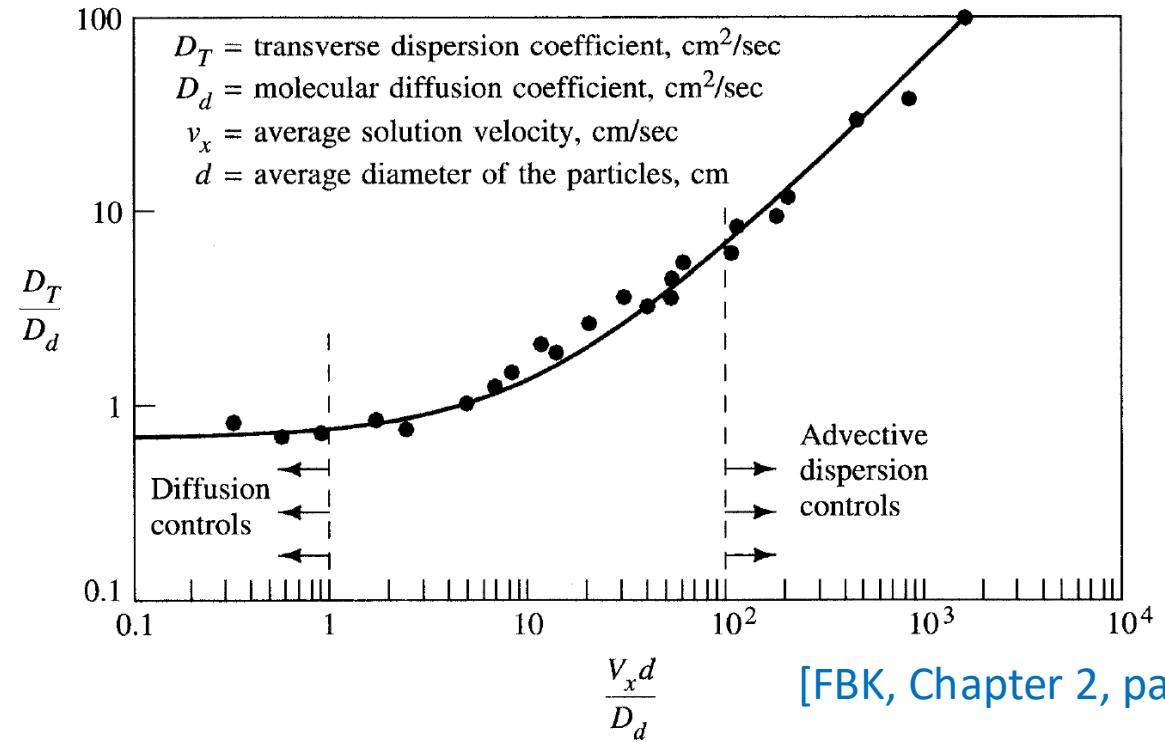
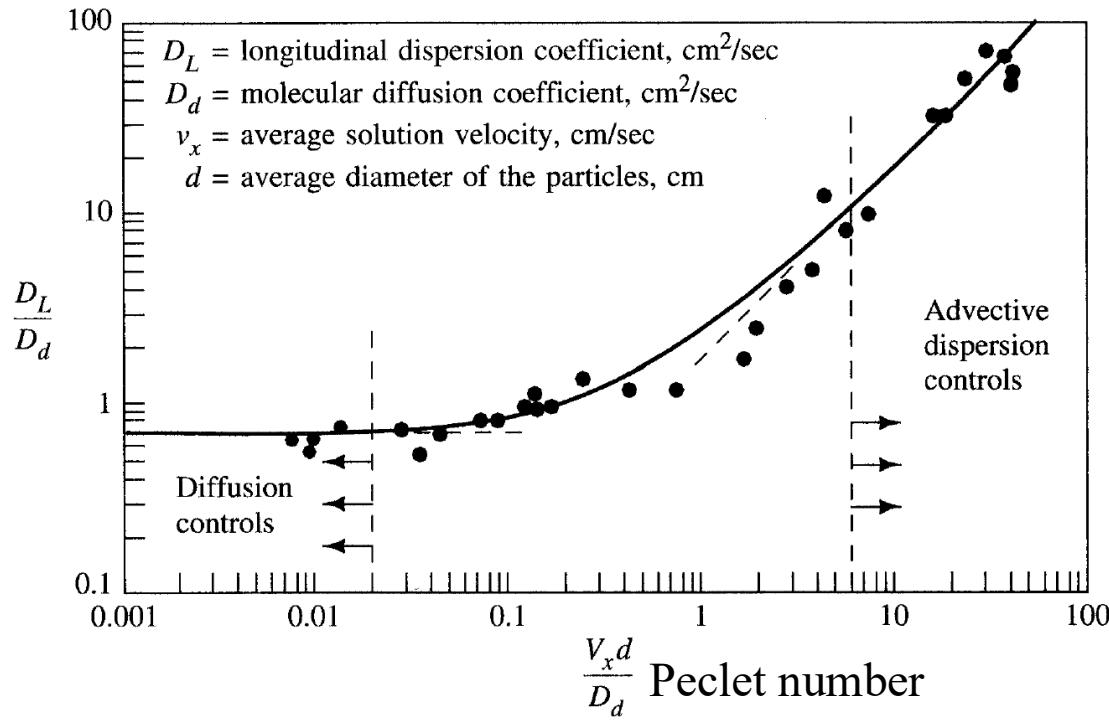
$$\Rightarrow \frac{\partial}{\partial t} (\phi c) + \nabla \cdot \underline{q}_c = 0$$

$$\underline{q}_c = \underline{q} c - \nu D \nabla c$$

$$\left. \begin{array}{l} \frac{\partial}{\partial t} (\phi c) + \nabla \cdot (\underline{q} c - \nu D \nabla c) = 0 \\ \end{array} \right\} \Rightarrow \boxed{\frac{\partial}{\partial t} (\phi c) + \nabla \cdot (\underline{q} c - \phi D \nabla c) = 0}$$

3D general equation for solute transport
in saturated porous media.

Solute transport under saturated flow



[FBK, Chapter 2, page 69]

- At lower Peclet numbers diffusion is the predominant force, and dispersion can be neglected
- At higher Peclet numbers mechanical dispersion is the predominant cause of mixing of the contaminant plume (Perkins and Johnson 1963; Bear 1972; Bear and Verruijt 1987) and the effects of diffusion can be ignored. Under these conditions D_i can be replaced with $a_i v_i$ in the advection-dispersion equations.
- In between, there is a transition zone, where the effects of diffusion and longitudinal mechanical dispersion are comparable.