HWRS 561b: Physical Hydrogeology II

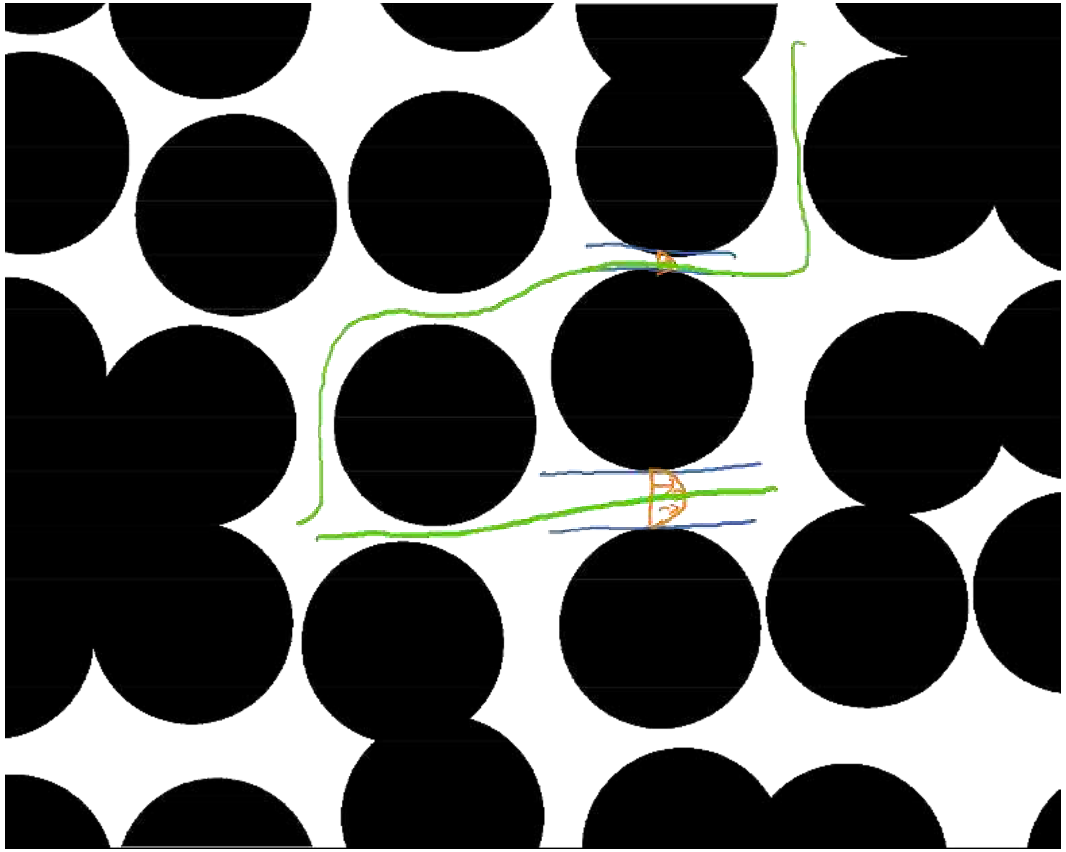
Solute transport (Part 2)

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

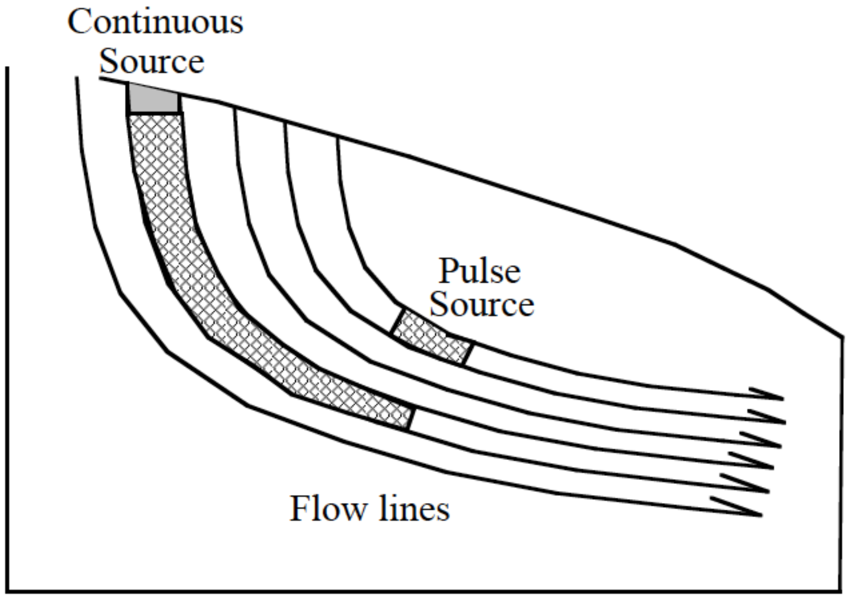


Spatial variation of velocity in a porous medium:

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

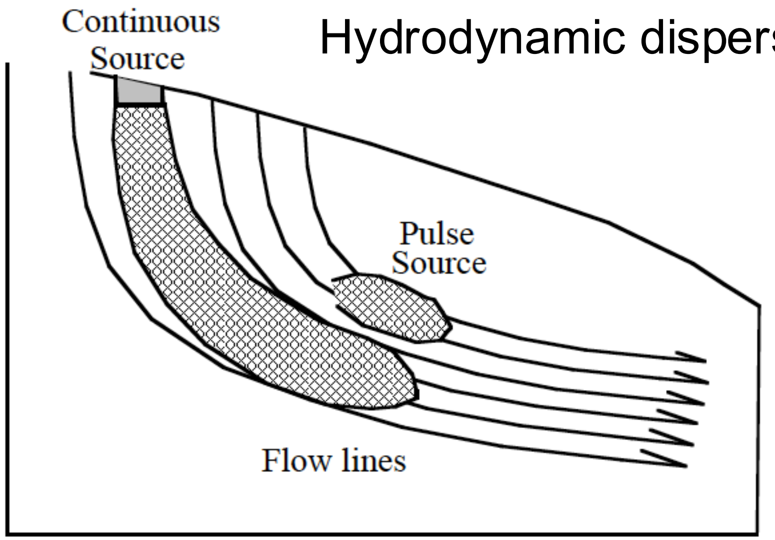
Solute transport under saturated flow

Pure advection



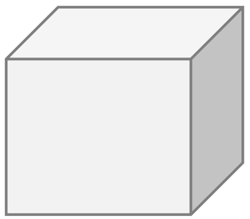
Advection + Mechanical dispersion + Molecular diffusion

Hydrodynamic dispersion

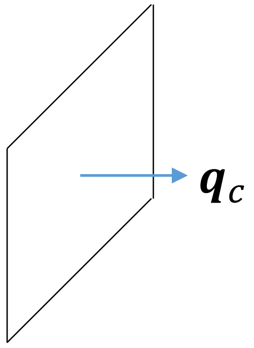


Solute transport under saturated flow

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

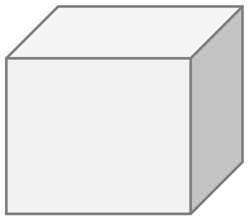


Saturated porous medium

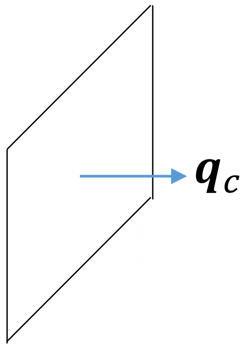


$$\boldsymbol{q}_c = \phi(\boldsymbol{v}C - \boldsymbol{D}\nabla C),$$

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



Fluid only
(e.g., free water)



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

Diffusion is isotropic, not a tensor.

Solute transport under saturated flow

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

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 $\mathbf{v}\mathbf{v}\cdot\mathbf{x} = \mathbf{v}(\mathbf{v}\cdot\mathbf{x})$

$$\boldsymbol{D} = \alpha_T|\boldsymbol{v}|\mathbf{I} + (\alpha_L - \alpha_T)\frac{\boldsymbol{v}\boldsymbol{v}}{|\boldsymbol{v}|} + wD_0\mathbf{I}$$

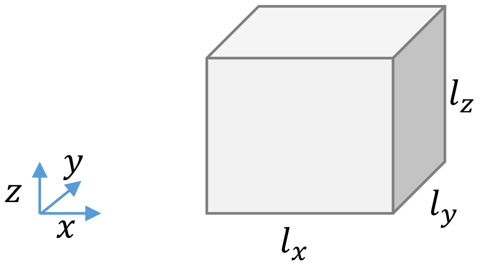
α_L and α_T are longitudinal and transverse dispersivities, respectively.

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

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

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

Solute transport under saturated flow



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

<u>Mass conservation</u>: 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:

$$-\int_\Omega \nabla\cdot\mathbf{q}_c\,dV = -\int_{\partial\Omega}\mathbf{q}_c\cdot\mathbf{n}\,dS \Leftarrow \left\{\begin{aligned} &\int_0^{l_y}\int_0^{l_z} q_{c,x}\Big|_{x=0} - \int_0^{l_y}\int_0^{l_z} q_{c,x}\Big|_{x=l_x} \\ &+\int_0^{l_x}\int_0^{l_z} q_{c,y}\Big|_{y=0} - \int_0^{l_x}\int_0^{l_z} q_{c,y}\Big|_{y=l_y} \\ &+\int_0^{l_x}\int_0^{l_y} q_{c,z}\Big|_{z=0} - \int_0^{l_x}\int_0^{l_y} q_{c,z}\Big|_{z=l_z} \end{aligned}\right.$$

Solute transport under saturated flow

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

$\Omega \neq \Omega(t)$

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

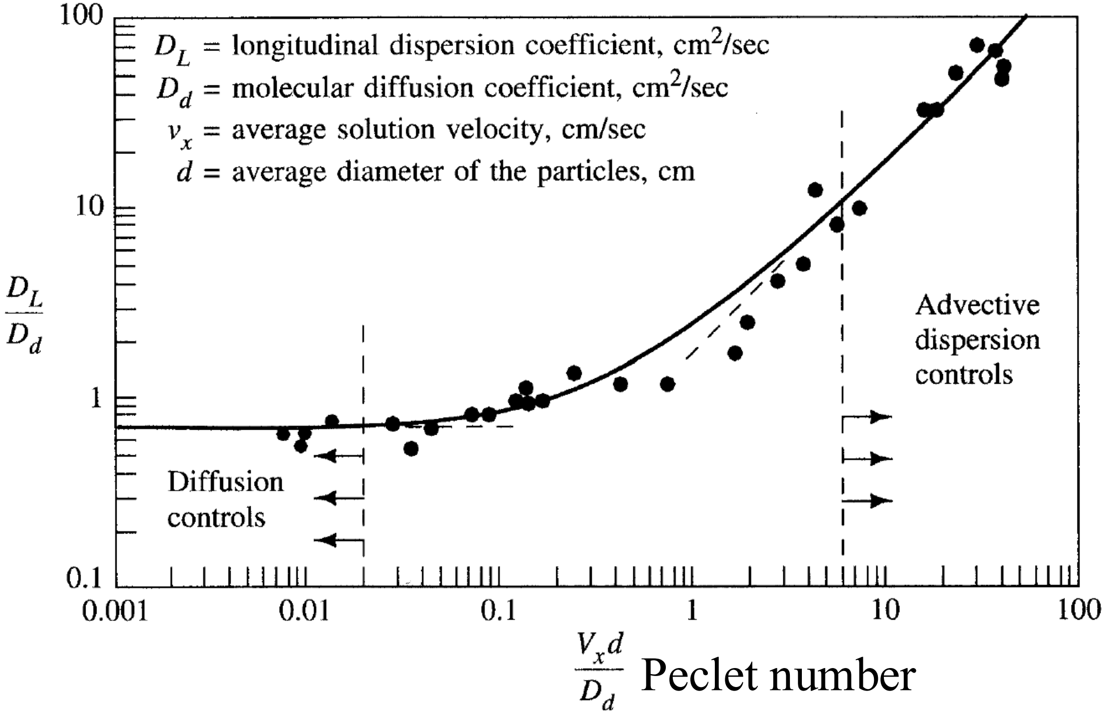
$$\Rightarrow \int_\Omega \left[\frac{\partial}{\partial t}(\phi c) + \underset{\sim}{\nabla}\cdot \underset{\sim}{q}_c\right] dv = 0$$

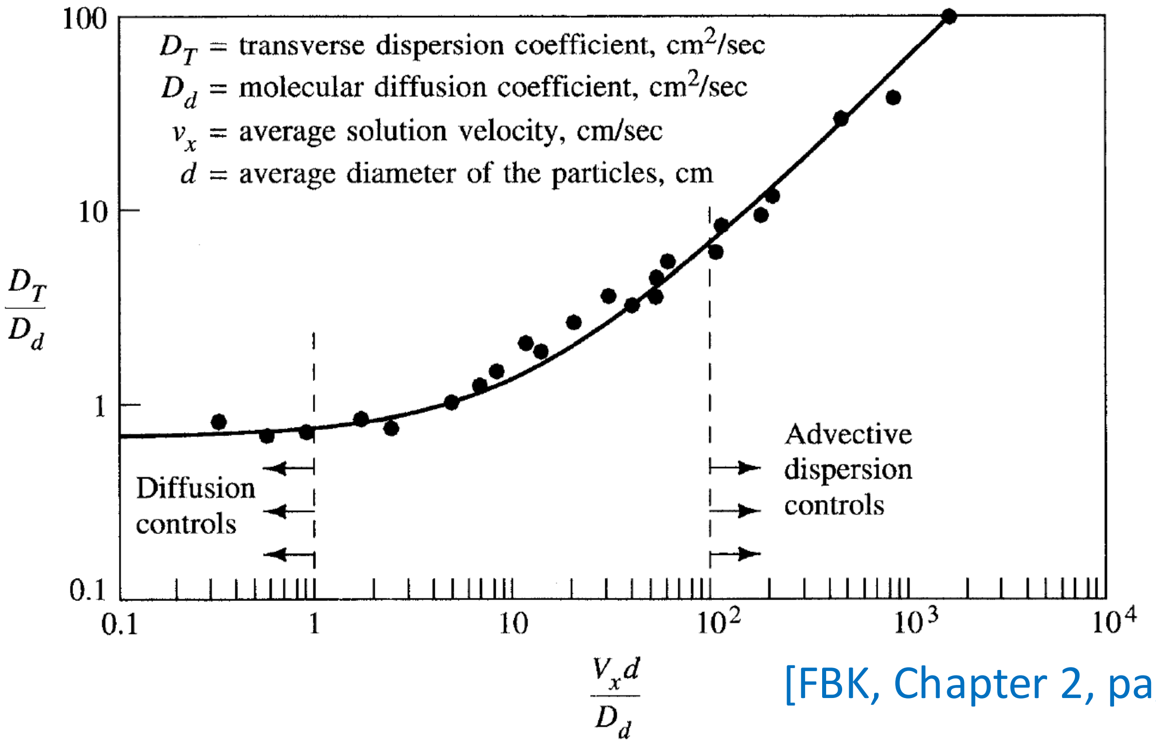
Ω is arbitrary

$$\Rightarrow \left.\begin{aligned} &\frac{\partial}{\partial t}(\phi c) + \underset{\sim}{\nabla}\cdot \underset{\sim}{q}_c = 0 \\ &\underset{\sim}{q}_c = \underset{\sim}{q}c - \phi \underset{\approx}{D}\underset{\sim}{\nabla} c \end{aligned}\right\} \Rightarrow \boxed{\frac{\partial}{\partial t}(\phi c) + \underset{\sim}{\nabla}\cdot\left(\underset{\sim}{q}c - \phi \underset{\approx}{D}\underset{\sim}{\nabla} c\right) = 0}$$

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.