HWRS 561b
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Spring 2026

HWRS 561b: Physical Hydrogeology II

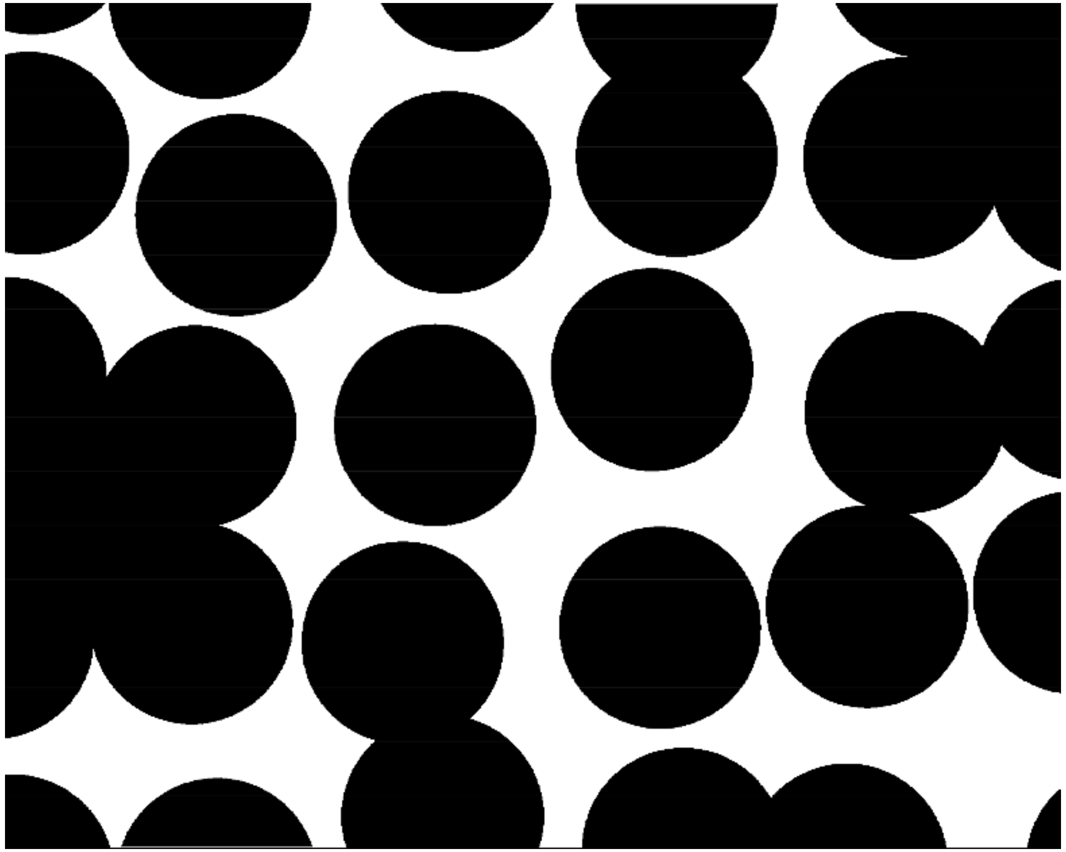
Solute transport (Part 2)

Agenda:

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

Solute transport under saturated flow

<u>Taylor-Aris Dispersion</u>: Spatial variation of velocity leads to dispersion of solutes

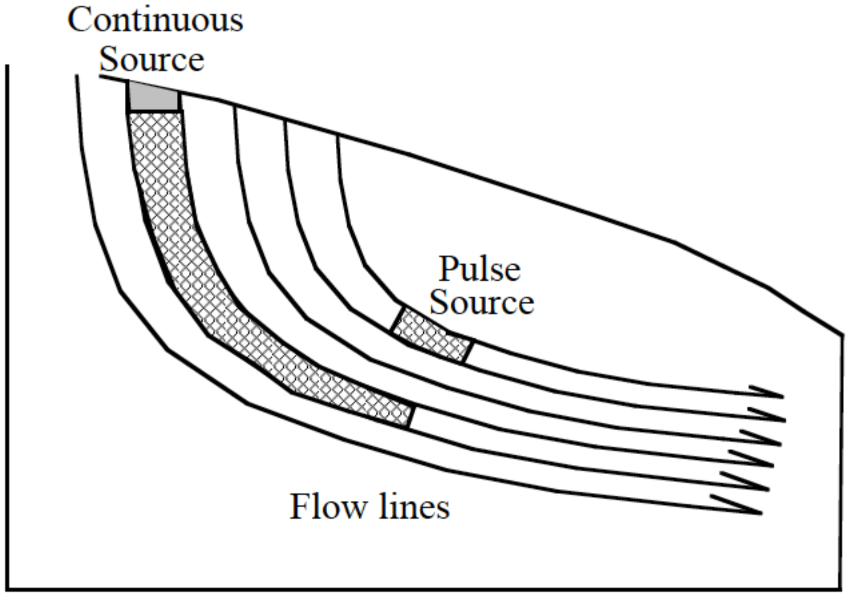


Spatial variation of velocity in a porous medium:

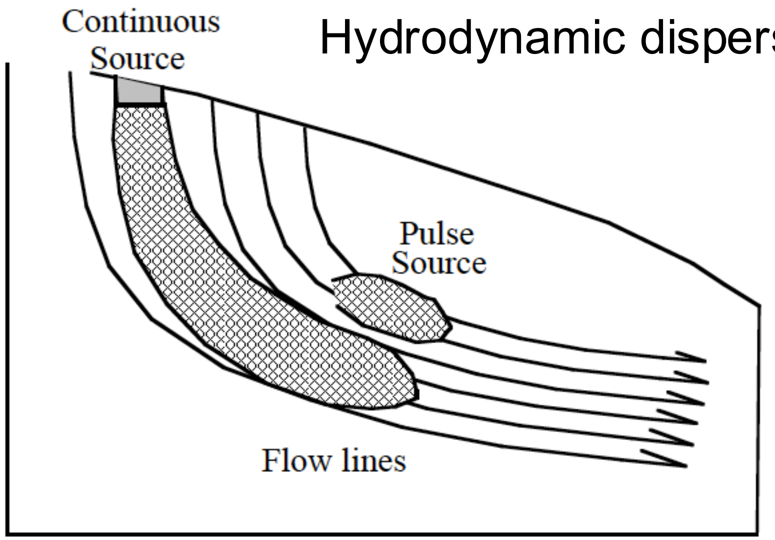
(1) Velocity profile through a pore throat (related to T-A dispersion)
(2) Velocity variation among pore throats
(3) Tortuosity

Solute transport under saturated flow

Pure advection

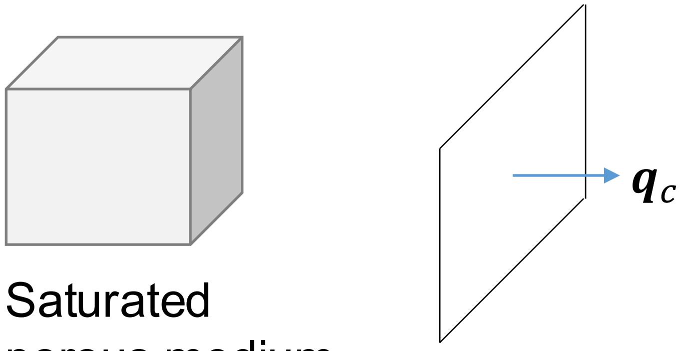


Advection + $\underbrace{\text{Mechanical dispersion + Molecular diffusion}}_{\text{Hydrodynamic dispersion}}$



Solute transport under saturated flow

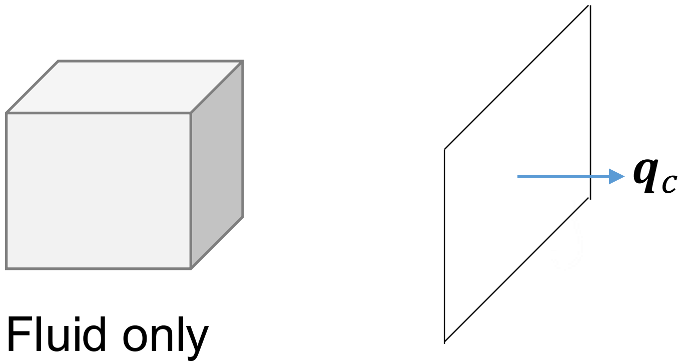
A widely used theory for describing solute flux in saturated porous media [J. Bear (1961)]



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

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

Outer product

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

α_L and α_T are longitudinal and transverse dispersivities, respectively.

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

$$q_x = \left[\alpha_T|\boldsymbol{v}| + (\alpha_L - \alpha_T)\frac{v_x^2}{|\boldsymbol{v}|} + wD_0\right]\frac{\partial C}{\partial x} + \left[(\alpha_L - \alpha_T)\frac{v_xv_y}{|\boldsymbol{v}|}\right]\frac{\partial C}{\partial y} + \left[(\alpha_L - \alpha_T)\frac{v_xv_z}{|\boldsymbol{v}|}\right]\frac{\partial C}{\partial z}$$

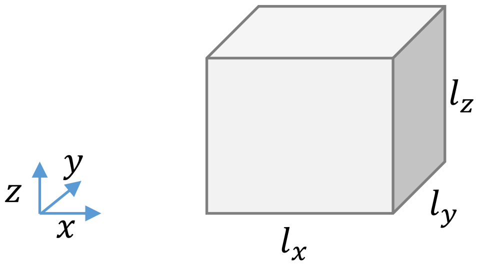
q_y and q_z can be written out in a similar way.

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

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

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

Solute transport under saturated flow



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

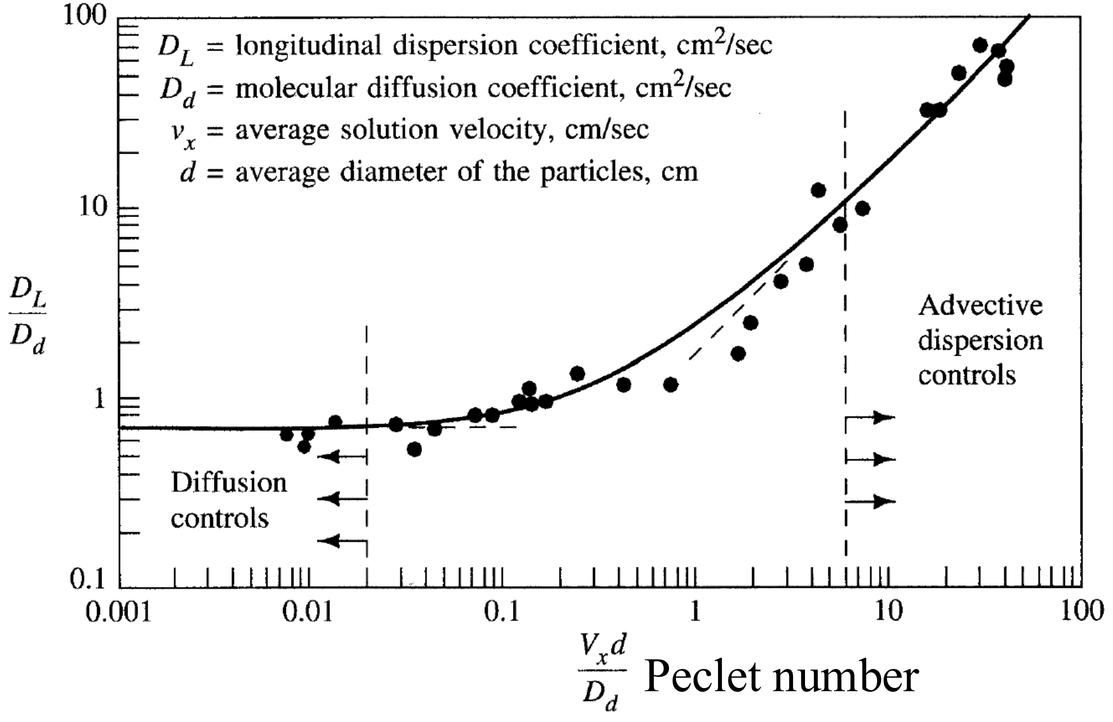
Mass conservation: Change of mass storage = mass in – mass out.

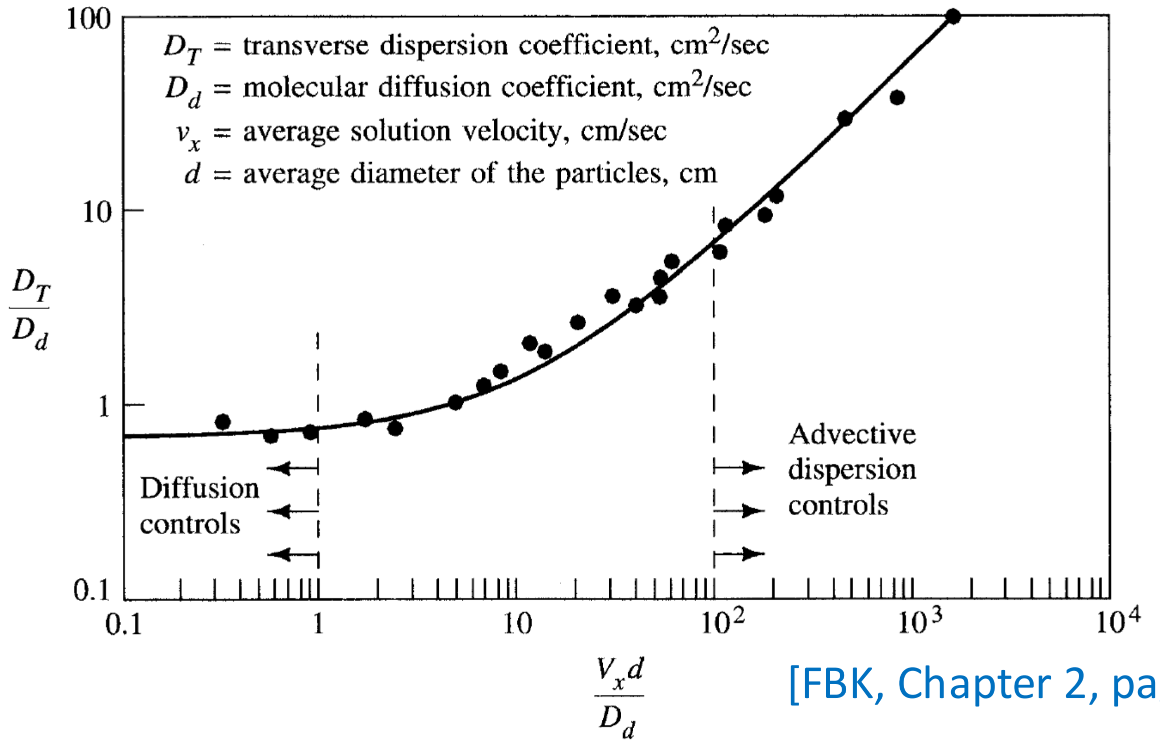
Rate of mass change:

Net fluxes:

Solute transport under saturated flow

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.