Lecture 16: Solute transport

Logistics: - HW5 is due (10/17)
- HW3 special deal if you complete over spring break just -15% late penalty!
- HW6 will be posted due Mar 21
  ⇒ Streamfunction

Last time: Correlated random fields
Properties: 1) correlation length
2) amplitude
3) mean

- Cov (X, Y)
- $C(\underline{h}) = \mathrm{Cov}(Z(\underline{x}), Z(\underline{x}+\underline{h}))$
  ⇒ controlls correlation length
- covariance models

Today: - Solute transport
- Advection-dissusion equation
- 2 new aspects: time derivative, advection

Solute Balance Equation

General balance equation: $\frac{\partial u}{\partial t} + \nabla \cdot \underline{j}(u) = \hat{f}(u)$

1) Define the unknown

- mass/mols of aqueous solute per unit volume of porous medium

$u \equiv \phi \rho X = \phi c$

X = mass/mole fraction $\frac{M}{M}$ $\frac{N}{N}$

ρ = density of fluid $\frac{M}{L^3}$

$c = \rho X$ = mass/molar conc. $\frac{M}{L^3}$ $\frac{N}{L^3}$

2) Define fluxes

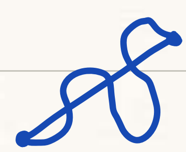
- Advective flux due to fluid flow

$\underline{j}_A = \underbrace{\phi \underline{v}}_{q} c = q c$ $\quad [1 \frac{L}{T} \frac{M}{L^3} = \frac{M}{L^2 T}]$

- Diffusive solute flux due to concentration gradients

Fick's law: $\underline{j}_D = -\tau \phi D_m \nabla c$ $\quad [1\; 1\; \frac{L^2}{T} \frac{1}{L} \frac{M}{L^3} = \frac{M}{L^2 T}]$

D_m = mol. diffusion coefficient $\frac{L^2}{T}$

τ = tortuosity < 1  1

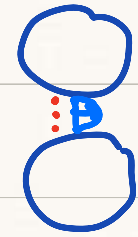
$D_m \approx 10^{-9} \frac{m^2}{s}$

- **Mechanical Dispersion:**

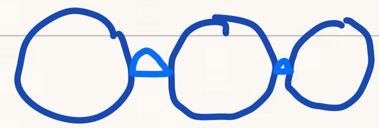
Def: Spreading of solutes due to variations in fluid velocity around the ave. velocity.

$\bar{\underline{v}} = \frac{q}{\phi}$ "mean interstitial velocity"

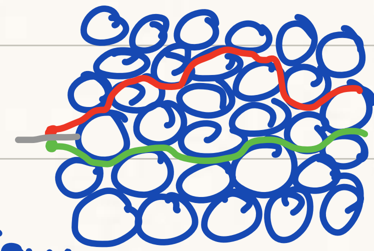
Causes: a) Velocity variation in single pore



b) Velocity variations between pores



c) Variation of length of path



Properties of mechanical dispersion:

1) Stronger in direction of flow weaker in the transverse direction $\Rightarrow$ anisotropic

2) Magnitude increases linearly with velocity/flux

Dispersion in 1D: $\boxed{D_d = \alpha_L q}$ $\quad L \frac{L}{T}$

α_L = longitudinal dispersivity [L]

in sphere pack: $\alpha_L \approx d$ ← grain diameter

Mechanical dispersion tensor

$$\boxed{\underline{\underline{D}}_M = (\alpha_L - \alpha_T)\frac{q \otimes q}{|q|} + \alpha_T |q| \underline{\underline{I}}}$$

α_L = long. dispersivity [L]
α_T = transverse dispersivity [L] $\alpha_T < \alpha_L$

Dyadic product: $q \otimes q = \begin{pmatrix} q_x \\ q_y \\ q_z \end{pmatrix} (q_x \; q_y \; q_z) = \begin{pmatrix} q_x^2 & q_x q_y & q_x q_z \\ q_y q_x & q_y^2 & q_y q_z \\ q_z q_x & q_z q_y & q_z^2 \end{pmatrix}$
Outer

Inner product: $q \cdot q = (q_x \; q_y \; q_z) \begin{pmatrix} q_x \\ q_y \\ q_z \end{pmatrix} = q_x^2 + q_y^2 + q_z^2$

Dispersive flux: $\boxed{\underline{j}_M = -\underline{\underline{D}}_M(q) \nabla c}$

3) Source term

Main interest in reactive transport

here simple example

$\hat{f} = -\phi k c$ k = reaction constant $\frac{1}{T}$

Solute balance:

substitute into general balance law

$$\boxed{\phi \frac{\partial c}{\partial t} + \nabla\cdot[\underline{q}\,c - (\tau\phi D_m + \underline{\underline{D}}_M(\underline{q}))\nabla c] = -\phi k c}$$

introduce $\underline{\underline{D}}_H(\underline{q}) = \tau\phi D_m + \underline{\underline{D}}_M(\underline{q})$

$$\boxed{\phi \frac{\partial c}{\partial t} + \nabla\cdot[\underline{q}\,c - \underline{\underline{D}}_H \nabla c] = -\phi k c}$$

Advection - Diffusion - Reaction Equ

Scaling of ADR equation

non-dimensionalize the variables

independent variables: x, t

dependent variable: $c(x,t)$, $\underline{q}(x,t)$ $D_H(x,t)$

pick 3 characteristic scales: x_c, t_c, c_c, q_c, D_c

dim. less variables: $x' = \frac{x}{x_c}$ $t' = \frac{t}{t_c}$ $c' = \frac{c}{c_c}$ $q' = \frac{q}{q}$

substitute: $\frac{\partial c}{\partial t} = \frac{\partial c_c c'}{\partial t_c t'} = \frac{c_c}{t_c}\frac{\partial c'}{\partial t'}$ $D_H' = \frac{D_H}{D_c}$

$$\frac{\phi \cancel{c_c}}{t_c}\frac{\partial c'}{\partial t'} + \frac{1}{x_c}\nabla'\cdot\left[q_c \cancel{c_c}\, q'c' - \frac{D_c \cancel{c_c}}{x_c} D_H' \nabla' c'\right] = \phi k \cancel{c_c} c'$$

$$\frac{\phi}{t_c}\frac{\partial c'}{\partial t'} + \nabla'\cdot\left[\frac{q_c}{x_c} q'c' - \frac{D_c}{x_c^2} D_H' \nabla' c'\right] = \phi k c'$$

Scale to accumulation term (time deriv)

$$\frac{\partial c'}{\partial t'} + \nabla'\cdot\left[\underbrace{\frac{q_c t_c}{\phi x_c}}_{\Pi_1} q'c' - \underbrace{\frac{D_c t_c}{\phi x_c^2}}_{\Pi_2} D_H' \nabla' c'\right] = \underbrace{k t_c}_{\Pi_3} c'$$

$\frac{1}{t_A}$ $\qquad \frac{1}{t_D}$ $\qquad \frac{1}{t_R}$

Π_1, Π_2, Π_3 are dimensionless groups

They suggest intrinsic time scales: $\qquad q = \phi v$

$\Pi_1 = \frac{q_c t_c}{\phi x_c} = 1 \Rightarrow t_c = \frac{x_c}{q_c/\phi} = \frac{x_c}{v_c} = t_A$ advective time

time to flow across distance x_c

$\Pi_2 = \frac{D_c t_c}{\phi x_c^2} = 1 \Rightarrow t_c = \frac{\phi x_c^2}{D_c} = t_D$ diffusion time

time to diffuse across distance x_c

$\Pi_3 = k t_c = 1 \Rightarrow t_c = \frac{1}{k}$ reaction time

time for c to decay

"e-folding time"

Have to pick one time scale

try to pick dominant process

Groundwater: advection $t_c = t_A$

$$\boxed{\frac{\partial c'}{\partial t'} + \nabla'\cdot\left[\frac{t_c}{t_A}\, \underline{q}'c' - \frac{t_c}{t_D}\, \underline{\underline{D}}'_H \nabla' c'\right] = \frac{t_c}{t_R}\, c'}$$

choose: $t_c = t_A$

$$\frac{\partial c'}{\partial t'} + \nabla'\cdot\left[\underline{q}'c' - \frac{t_A}{t_D}\, \underline{\underline{D}}'_H \nabla' c'\right] = \frac{t_A}{t_R}\, c'$$

Peclet number: $Pe = \frac{t_D}{t_A} = \frac{\cancel{\phi}\, x_c^2}{D_c}\,\frac{q_c}{x_c \cancel{\phi}} = \frac{q_c x_c}{D_c}$

compares diffusive & advective transport

$Pe \gg 1$ advection dominates

$Pe \ll 1$ diffusion dominates

$$\frac{\partial c'}{\partial t'} + \nabla'\cdot\left[\underline{q}'c' - \frac{1}{Pe}\, \underline{\underline{D}}'_H \nabla' c'\right] = Da\, c'$$

Da = Damkohler number $= \frac{t_A}{t_R}$

$t_c = t_D$

$$\frac{\partial c}{\partial t} + \nabla \cdot \left[Pe \, \underline{q} c - D_H \nabla c \right] = \dots c$$

$Pe \, Da$