Tutorial II: Dispersion and methods of moments

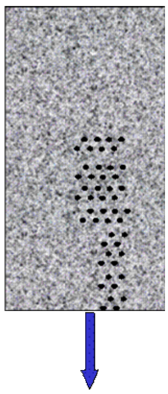
1 Measuring transport distance: We perform tracer experiments in the field and measure the concentration as a function of depths at a fixed time.

- What are the main ideas in the method of moments to estimate the Dispersion coefficient?
- What is the transport distance pdf?
- Describe the first and second moment with your own words.

The analytical solution in case of a constant water flux, homogeneous semi-infinite soil and a Dirac puls as initial condition.

$$\frac{\theta}{m_0} C_w(z, t_c) = \frac{1}{(4\pi Dt)^{1/2}} \exp\left(-\frac{(z - vt_c)^2}{4Dt_c} \right)$$
$$\mathrm{t_c} = \text{const.}$$

- Why does the soil moisture pop up in the equation?
- What happens to the first moment and second moment when we increase D?
- What happens to the first moment and second moment when we increase v?
- What happens to the first moment and second moment when we increase tc?
- How could we account for degradation in this most simple model?



2 Measuring transport times: We perform tracer breakthrough experiments in the field and measure the concentration as a function of depths at a fixed time.

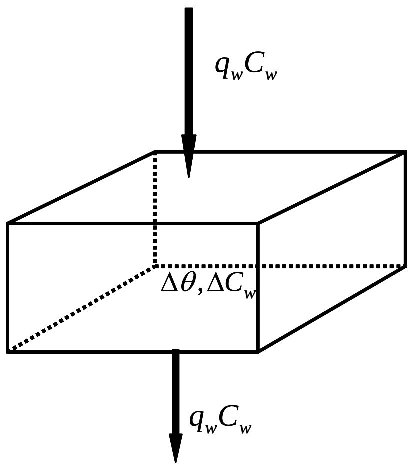
- What is the statistical analogue to the transport distance pdf? How to define it?
- What is the first and second moment in your own words?
- How to estimate the Dispersion coefficient?

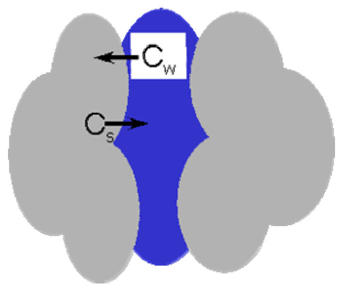
The analytical solution in case of a constant water flux, homogeneous soil and a Dirac puls as initial condition and for large Peclet numbers is.

$$\frac{q_w}{m_0} C_f(L,t) = \frac{L}{\left(4\pi D\left(\frac{L}{v}\right)^3\right)^{1/2}} \exp\left(-\frac{\left(t - L/v\right)^2}{4D\, L/v^3}\right)$$

C^f is the flux averaged concentration q_s/q_w

- What happens to the first moment and second moment when we increase D?
- What happens to the first moment and second moment when we increase v?
- What happens to the first moment and second moment when we increase L?
- How is D related to the second moment of the transport time pdf?





q_w, water flux
C_w, concentration in water phase [kg/m^3].
Cs concentration in adsorbed phase [kg/m^3]
Cs mass specific concentration in adsorbed phase [kg/kg]

3 Outlook to Transport of adsorbing solutes:
Derive a mass balance equation for an instantaneously adsorbing solute!

$$\rho C_t = C_s$$

$$\frac{k_{ad}}{\rho k_{des}} = K_d = \frac{C_t}{C_w}$$

Eliminate the concentration in the adsorbed phase from this equation. What could be the use?

4 Outlook to numerical methods: particle tracking for simulating solute transport.

Represent the total solute mass M in the soil as by N particles with mass M/N. Simulate solute transport as superposition of deterministic advection step and diffusive step within a time step Δt. R is pseudo-random number, uniformly distributed between [-1, 1].
What is the asymptotic distribution of travel distance for a large number of N and times much larger than Δt (think of the central limit theorem CLT)?

$$z(t+\Delta t) = z(t) + v\Delta t \pm R\sqrt{6D\Delta t}$$

What to we need to build a simple numerical model based on particle tracking?
v Transport velocity
D Dispersion coefficient
Random number generator

Literature

- Roth, K. and Hammel, K. (1996): Transport of a conservative chemical through an unsaturated two-dimensional Miller-similar medium with steady state flow. Water Resour. Res. 32 (6): 1653 – 1663.
- KINZELBACH, W. AND UFFINK, G. (1991): The random walk method and extensions in groundwatermodeling. In: Transport Processes in Porous Media, Bear J. et al. (eds.), Kluwer (NATO ASI series E 202)

Solution 2

$$h(\Delta t_i) = \frac{1}{\Delta t_i}\frac{n(L,t_i)\mu}{n_0\mu} = \frac{q_w C_f(L,\Delta t_i)}{m_0} = \frac{q_s L,\Delta t_i)}{m_0}$$

$$\sum_i h(\Delta t_i)\Delta t_i = 1$$

h = relative frequency t
qw = soil water flow
μ= Molecule mass [kg]

$$\bar{t} = \sum_i t_i h(t_i)\Delta t_i = \sum_i t_i \frac{q_w C_f(L,\Delta t_i)}{m_0}\Delta t_i$$

$$\mathrm{var}(t) = \sum_i (t_i - \bar{t})^2 h(t_i)\Delta t_i = \sum_i (t_i - \bar{t})^2 \frac{q_w C_j(L,\Delta t_i)}{m_0}\Delta t_i$$

$$\frac{q_w}{m_0} C_f(L,t) = \frac{L + vt}{4(\pi D t^3)^{1/2}} \exp\left(-\frac{\left(t - L/v\right)^2}{4D\ t/v^2}\right)$$

$$D = \frac{1}{2}\frac{v^3\,\mathrm{var}(t)}{L} = \frac{1}{2}\frac{v^3 \sum_i \frac{q_w C^w_{av}(t_i, L)}{m_0}\Delta t_i \left(t_i - \frac{L}{v}\right)^2}{L}$$

$$\frac{\partial(\theta C_w + \rho C_t)}{\partial t} = q_{wasser}\frac{\partial(C_w)}{\partial z} - \frac{\partial}{\partial z}\left(D\frac{\partial C_w}{\partial z}\right)$$

$$\theta\frac{\partial(C_w + \rho/\theta\, C_t)}{\partial t} = q_{wasser}\frac{\partial(C_w)}{\partial z} - \frac{\partial}{\partial z}\left(D\frac{\partial C_w}{\partial z}\right)$$