HWRS 561b: Physical Hydrogeology II

Solute transport (Part 3)

Agenda:

1. Analytical solutions for solute transport
2. Scale effects of dispersion

Simplified 1D advection-dispersion equation

3D governing equation for solute transport in saturated porous media

$$\frac{\partial}{\partial t}(\phi C) + \nabla \cdot (\mathbf{q}C - \phi \mathbf{D}\nabla C) = 0$$

1D simplification (assuming constant porosity in space)

$$\frac{\partial C}{\partial t} + \frac{\partial}{\partial x}\left(VC - D\frac{\partial C}{\partial x}\right) = 0$$

1) $\div \phi$
2) $V = V_x$
3) $D = D_{xx}$

Assuming constant porewater velocity and dispersion coefficient, we obtain

$$\frac{\partial C}{\partial t} + V\frac{\partial C}{\partial x} - D\frac{\partial^2 C}{\partial x^2} = 0$$

Simplified 1D advection-dispersion equation

$$\frac{\partial C}{\partial t} + V\frac{\partial C}{\partial x} - D\frac{\partial^2 C}{\partial x^2} = 0$$

Note:
1) This is a second-order partial differential equation.
2) It is linear, e.g., coefficients does not depend on *C*.
3) It can be solved analytically, i.e., we can obtain a close-form solution for *C* for any *x* and *t.*

To solve the 1D equation, we need to specify one initial condition and two boundary conditions.

First-order in time.

Second-order in space.

Non-dimensional form and dimensionless number

Define $\tilde{x} = \frac{x}{L}$, $\tilde{t} = \frac{t}{L/V}$, $\tilde{C} = \frac{C}{C_0}$

$$\frac{\partial C}{\partial t} = \frac{\partial(\tilde{C} C_0)}{\partial(\tilde{t}\, L/V)} = \frac{V C_0}{L}\frac{\partial \tilde{C}}{\partial \tilde{t}}$$

$$V\frac{\partial C}{\partial x} = V\frac{\partial(\tilde{C} C_0)}{\partial(\tilde{x} L)} = \frac{V C_0}{L}\frac{\partial \tilde{C}}{\partial \tilde{x}}$$

$$D\frac{\partial^2 C}{\partial x^2} = D\frac{\partial^2(\tilde{C} C_0)}{\partial(\tilde{x} L)^2} = \frac{D C_0}{L^2}\frac{\partial^2 \tilde{C}}{\partial \tilde{x}^2}$$

$$\frac{V C_0}{L}\frac{\partial \tilde{C}}{\partial \tilde{t}} + \frac{V C_0}{L}\frac{\partial \tilde{C}}{\partial \tilde{x}} - \frac{D C_0}{L^2}\frac{\partial^2 \tilde{C}}{\partial \tilde{x}^2} = 0$$

$$\Rightarrow \frac{\partial \tilde{C}}{\partial \tilde{t}} + \frac{\partial \tilde{C}}{\partial \tilde{x}} - \frac{D}{VL}\frac{\partial^2 \tilde{C}}{\partial \tilde{x}^2} = 0$$

Define $Pe \equiv \frac{VL}{D}$

$$\frac{\partial \tilde{C}}{\partial \tilde{t}} + \frac{\partial \tilde{C}}{\partial \tilde{x}} - \frac{1}{Pe}\frac{\partial^2 \tilde{C}}{\partial \tilde{x}^2} = 0$$

physical meaning:

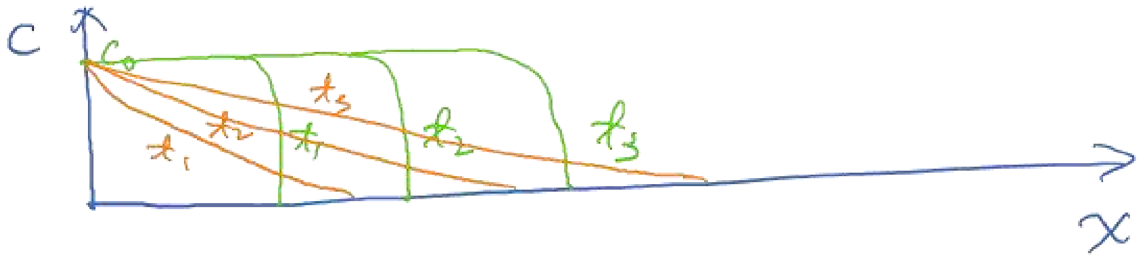
$$Pe = \frac{\text{Advective transport rate}}{\text{Dispersive transport rate}} = \frac{\text{Dispersive time scale}}{\text{Advective time scale}}.$$

$$\left.\begin{aligned} t_{Adv} &= L/V \\ t_{Disp} &= L^2/D \end{aligned}\right\} \Rightarrow Pe = \frac{L^2/D}{L/V} = \frac{VL}{D}$$

① $Pe \gg 1$: Advection-dominated
② $Pe \ll 1$: Dispersion-dominated
③ $Pe \sim O(1)$: Balanced.

1D step change in concentration

Let us first consider a semi-infinite domain.



Initial condition

$$C(x,0) = 0,\ x \geq 0$$

Boundary conditions (assuming semi-infinite domain)

$$C(0,t) = C_0,\ t \geq 0$$

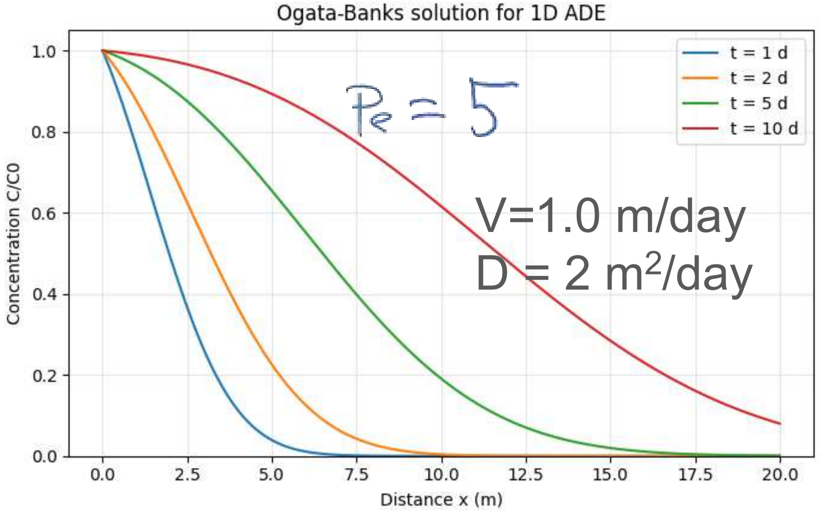
$$C(\infty,t) = 0,\ t \to \infty$$

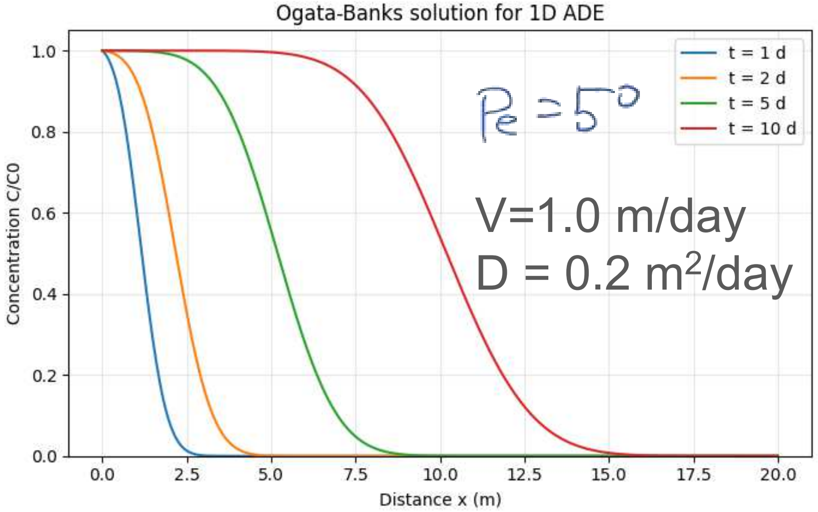
$$C = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) + \exp\left(\frac{Vx}{D}\right)\operatorname{erfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right]$$

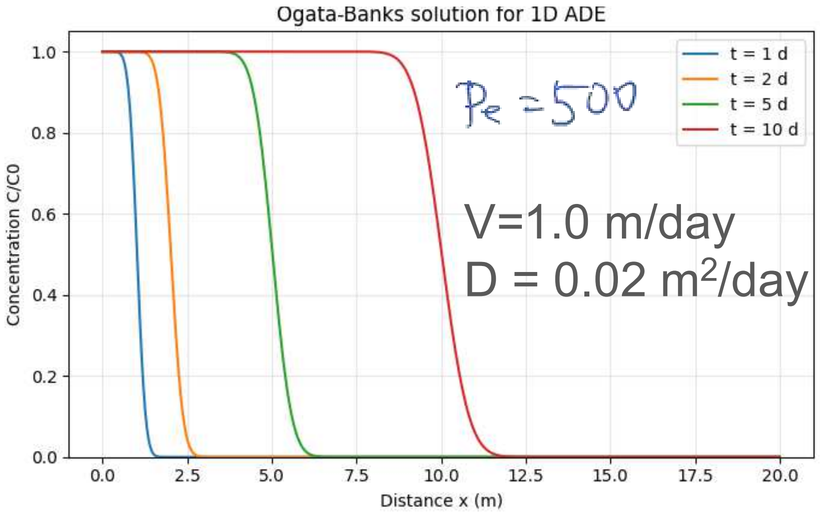
[Ogata and Banks, 1961]

1D step change in concentration

$$C = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) + \exp\left(\frac{VL}{D}\right)\operatorname{erfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right]$$







$Pe = \frac{VL}{D}$

$L = 10$

1D step change in concentration

Gaussian distribution

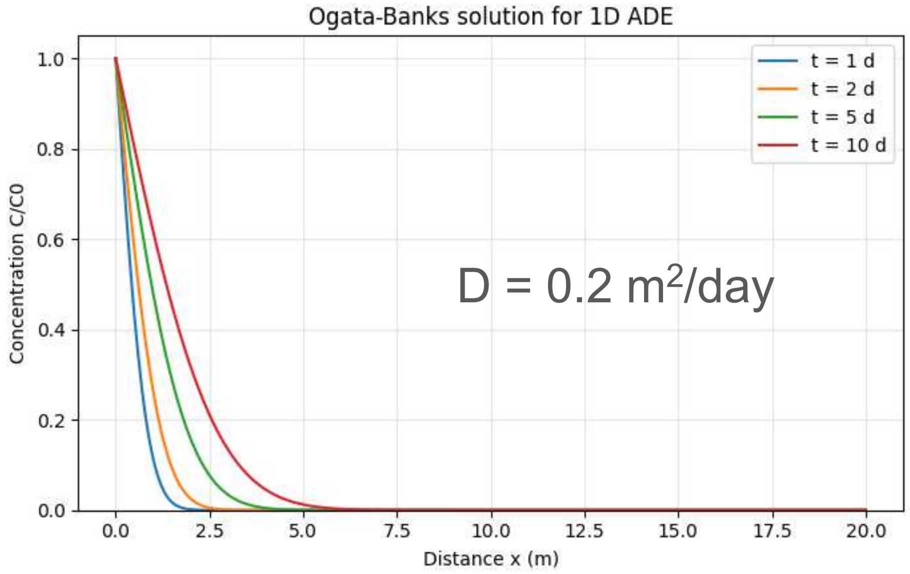
PDF $\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

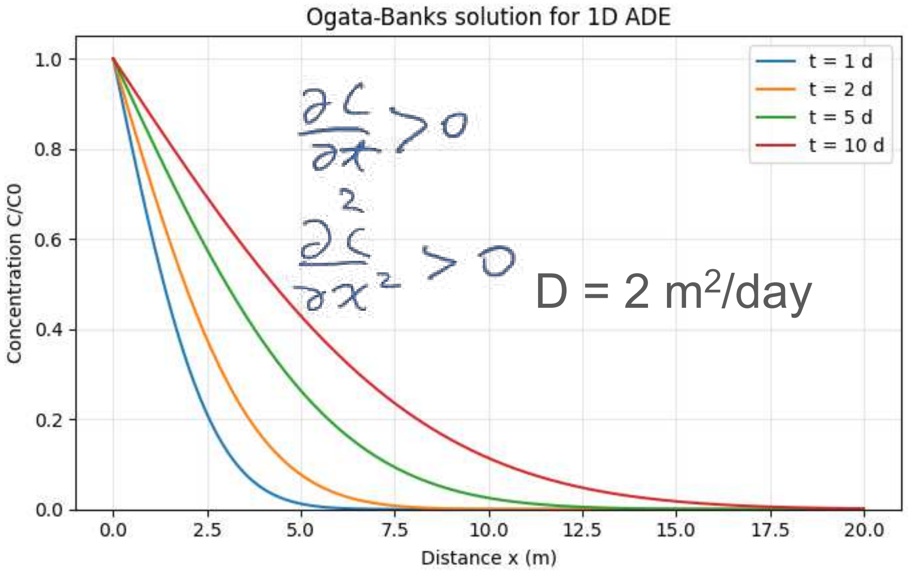
CDF $\Phi\left(\frac{x-\mu}{\sigma}\right) = \frac{1}{2}\left[1 + \mathrm{erf}\left(\frac{x-\mu}{\sigma\sqrt{2}}\right)\right]$

Special case: *V=0* (only dispersion)

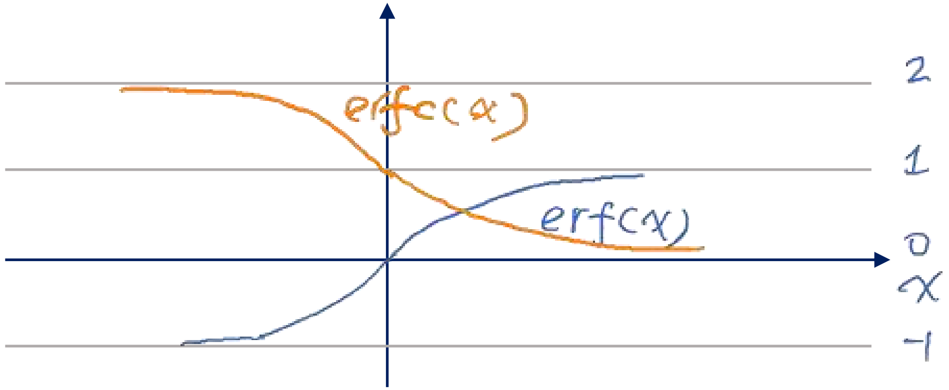
$$C = C_0 \,\mathrm{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$





$$\mathrm{erfc}(x) = 1 - \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}\,dt = 1 - \mathrm{erf}(x)$$



1D step change in concentration

Characteristic time scales for advection and dispersion

[Scaling analysis]

Advection Equation:

$$\frac{\partial c}{\partial t} = -V\frac{\partial c}{\partial x} \qquad c \sim c_0, \; t \sim t_c, \; x \sim x_c$$

$$\Rightarrow \frac{c_0}{t_c} \sim V\frac{c_0}{x_c}$$

$$\Rightarrow t_c \sim \frac{x_c}{V} = \frac{L}{V} \qquad [\text{let } L = x_c]$$

Dispersion Equation:
(Diffussion)

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2}$$

$$\frac{c_0}{t_c} \sim D\frac{c_0}{x_c^2} \Rightarrow t_c \sim \frac{x_c^2}{D} = \frac{L^2}{D}$$

"Baking turkey"

Heating is governed by

$$\frac{\partial T}{\partial t} = \alpha\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right)$$

heat conductivity

$$\frac{T_0}{t_c} \sim \alpha\frac{1}{r_c^2}\frac{r_c^2}{r_c^2}T_0$$

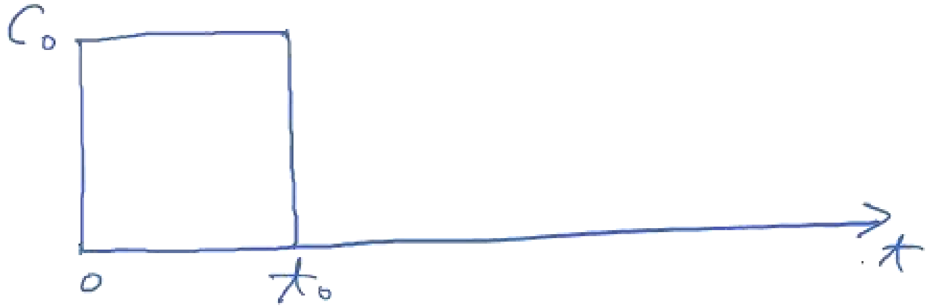
$$\Rightarrow t_c \sim \frac{r_c^2}{\alpha}$$

"Turkey twice big requires four times baking time"

1D pulse change in concentration

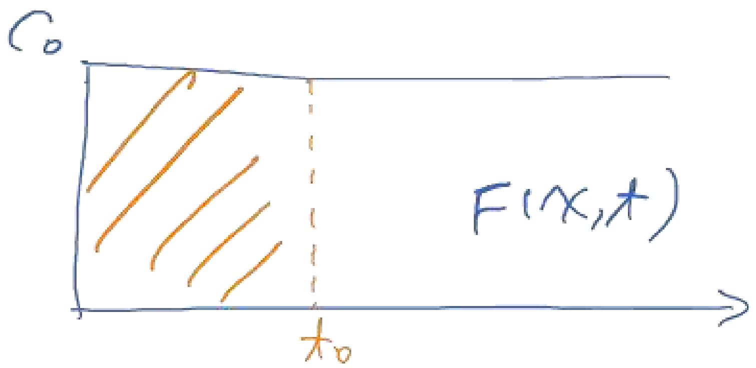
Pulse change in concentration

$$C(0,t) = C_0,\ 0 \le t \le t_0$$
$$C(0,t) = 0,\ t \ge t_0$$



Let the solution for the step change be $(t \ge t_0)$

$$F(x,t) = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x-Vt}{2\sqrt{Dt}}\right) + \exp\left(\frac{Vx}{D}\right)\operatorname{erfc}\left(\frac{x+Vt}{2\sqrt{Dt}}\right)\right]$$



Then, the solution for pulse change can be written as

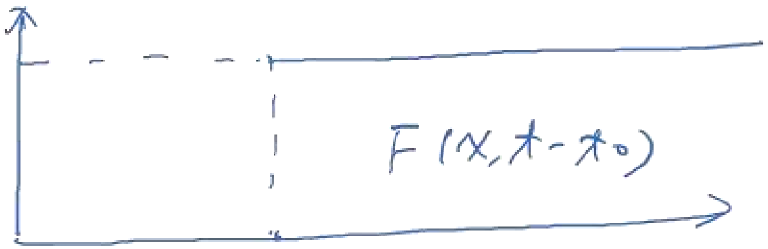
$0 \le t < t_0$

$$C = F(x,t)$$

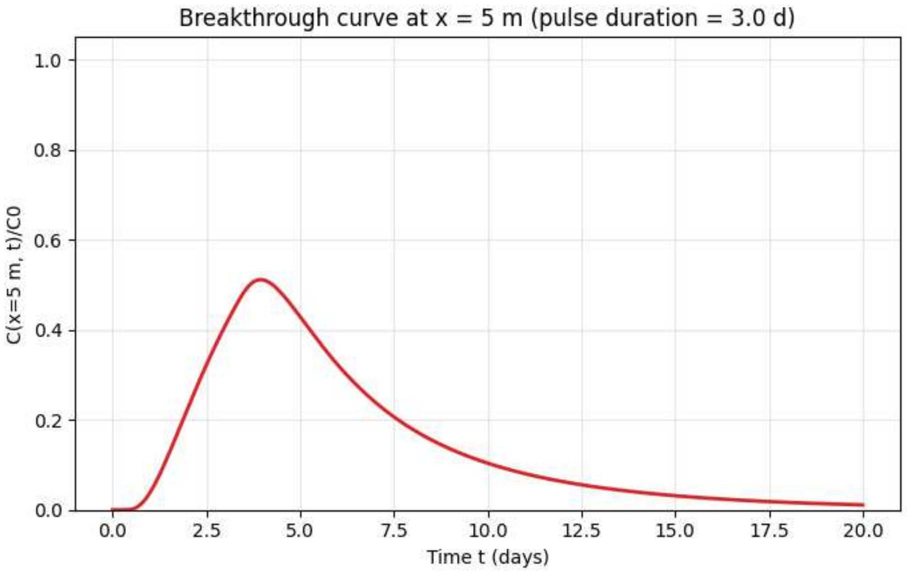
$t \ge t_0$

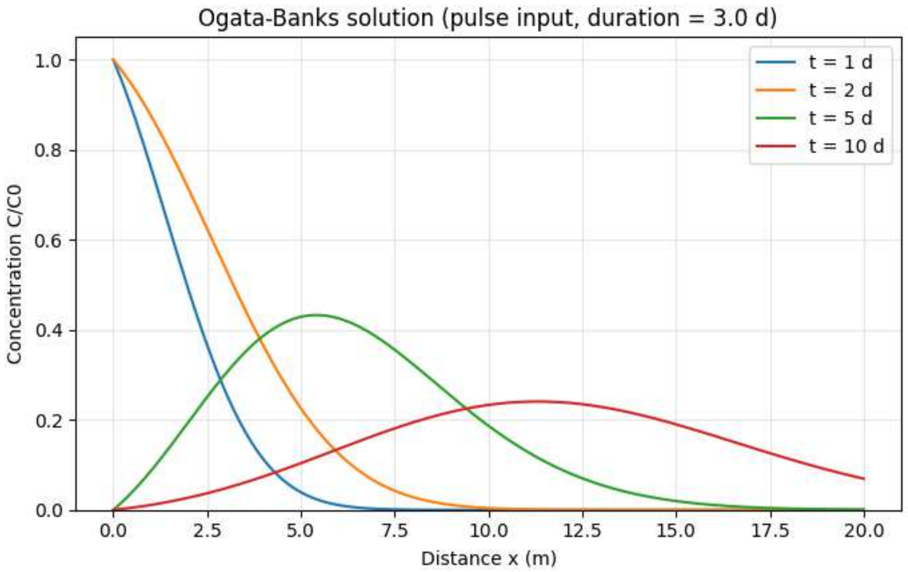
$$C = F(x,t) - F(x,t-t_0)$$

Subtract the solution for step change starting at t_0.



Moment analysis





Pulse injection

$$C(0,t) = C_0,\ 0 \le t \le t_0$$
$$C(0,t) = 0,\ t \ge t_0$$
$$t_0 = 3\,\mathrm{d}$$

$$M_t^0 = \int_0^\infty C\,dt$$

Total mass passing the observation point.

$$M_s^0 = \int_0^\infty C\,dx$$

Total mass in the system at a given time.

$$M_t^1 = \frac{\int_0^\infty C\,t\,dt}{\int_0^\infty C\,dt} = \frac{\int_0^\infty C\,t\,dt}{M_t^0}$$

Arrival time

$$M_x^1 = \frac{\int_0^\infty C\,x\,dx}{\int_0^\infty C\,dx} = \frac{\int_0^\infty C\,x\,dx}{M_x^0}$$

Center of mass

$$M_{t,adj}^1 = \frac{\int_0^\infty C\,t\,dt}{M_t^0} - \frac{1}{2}T_0$$

Travel time

(T_0 is the pulse duration)

Moment analysis

TABLE 2.2 One-dimensional moments.

Moment	Temporal Moments		Spatial Moments	
Zeroth Absolute Moment	$M_t^0 = \int_0^\infty C\,dt$	Total mass passing the observation point.	$M_s^0 = \int_0^\infty C\,dx$	Total mass in the system at a given time.
First Normalized Moment	$M_t^1 = \dfrac{\int_0^\infty Ct\,dt}{\int_0^\infty C\,dt} = \dfrac{\int_0^\infty Ct\,dt}{M_t^0}$	Arrival time	$M_s^1 = \dfrac{\int_0^\infty Cx\,dx}{\int_0^\infty C\,dx} = \dfrac{\int_0^\infty Cx\,dx}{M_x^0}$	Center of mass
Adjusted First Temporal Moment	$M_{adj}^1 = \dfrac{\int_0^x Ct\,dt}{M_t^0} - \dfrac{1}{2}T_0$	Travel time (T_0 is the pulse duration)	Not defined	
Second Central Moment	$M_t^2 = \dfrac{\int_0^\infty \left(t - M_t^1\right)^2 C\,dt}{M_t^0}$	Temporal variance	$M_s^2 = \dfrac{\int_0^\infty \left(x - M_s^1\right)^2 C\,dx}{M_s^0}$	Spatial variance
Third Central Moment	$M_t^3 = \dfrac{\int_0^\infty \left(t - M_t^1\right)^3 C\,dt}{M_t^0}$	Skewness of arrival times	$M_s^3 = \dfrac{\int_0^\infty \left(x - M_s^1\right)^3 C\,dx}{M_s^0}$	Plume asymmetry in space
Fourth Central Moment	$M_t^4 = \dfrac{\int_0^\infty \left(t - M_t^1\right)^4 C\,dt}{M_t^0}$	Tailedness (kurtosis) of the breakthrough curve	$M_s^4 = \dfrac{\int_0^\infty \left(x - M_s^1\right)^4 C\,dx}{M_s^0}$	Plume intermittency and extreme spreading

Moment analysis

- First normalized moment can be used to determine velocity (assuming no retardation)

$$M_t^1 = x/V$$

Note: The first normalized moment is not related to dispersion.

- The second temporal moment and second spatial moment are the temporal and spatial variances, which can both be used to determine the dispersion coefficient.

$$M_t^2 = \frac{\int_0^\infty \left(t - M_t^1\right)^2 C\,dt}{M_t^0} = 2DL/v^3 \Rightarrow D = \frac{v^3}{2x} M_t^2$$

(e.g. from expts)
Given the breakthrough cure, we can estimate the dispersion coefficient.

$$M_s^2 = \frac{\int_0^\infty \left(x - M_x^1\right)^2 C\,dx}{M_s^0} = 2Dt \Rightarrow D = \frac{M_s^2}{2t}$$

Given the plume shape, we can estimate the dispersion coefficient.

Continuous injection (3rd-type boundary condition)

Initial condition

$$C(x,0) = 0,\; x \geq 0$$

Boundary conditions (assuming semi-infinite domain)

$$\left(-D\frac{\partial C}{\partial x} + VC\right)\Bigg|_{x=0} = VC_0$$

$$\frac{\partial C}{\partial x}\Bigg|_{x\to\infty} = \text{(finite)}$$

$$C = \frac{C_0}{2}\left[\operatorname{erfc}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) + \left(\frac{V^2 t}{\pi D}\right)^{1/2}\exp\left(-\frac{(x-Vt)^2}{4Dt}\right)\right.$$
$$\left. -\frac{1}{2}\left(1 + \frac{Vx}{D} + \frac{V^2 t}{D}\right)\exp\left(\frac{Vx}{D}\right)\operatorname{erfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right]$$

Similar to the step change case, we can construct the solution for a pulse injection using superposition.

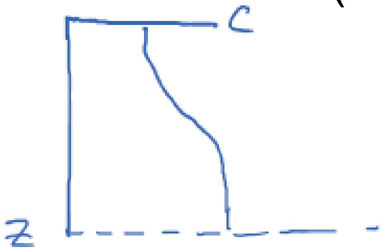
[van Genuchten, 1981]

Continuous injection (3rd-type boundary condition)

The solution is for a semi-infinite domain. If we want to use it for a finite domain (e.g., column experiments), we need to modify the solution.

For a column experiment, we typically do not know the boundary condition at the outlet. Often, we assume that the gradient of concentration is zero (i.e., dispersive flux is zero).

$$\left.\frac{\partial C}{\partial x}\right|_{x=L} = 0$$



This will not be the case for solution for a semi-infinite domain. Thus, if we want to use the semi-infinite domain solution to model the column experiment, we need to do the following

$$\left.\left(-D\frac{\partial C}{\partial x} + VC\right)\right|_{x=L} = VC_f$$

where *Cf* is the flux-based concentration as if there is no dispersive flux, i.e., all of the flux occurs as advection.

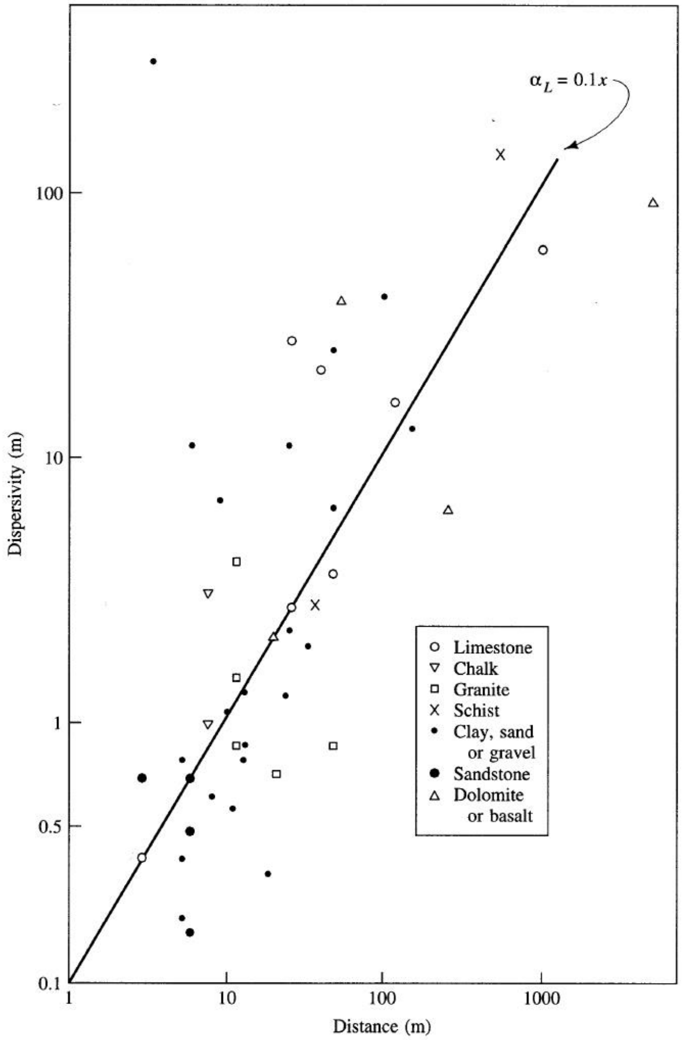
Substituting the solution for the volume-based concentration (from previous slide), we obtain the flux-based concentration

$$\frac{C_f(x,t)}{C_0} = \frac{1}{2}\left[\operatorname{erfc}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) + \exp\left(\frac{Vx}{D}\right)\operatorname{erfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right]$$

[van Genuchten, 1981]

Scale effects of dispersion

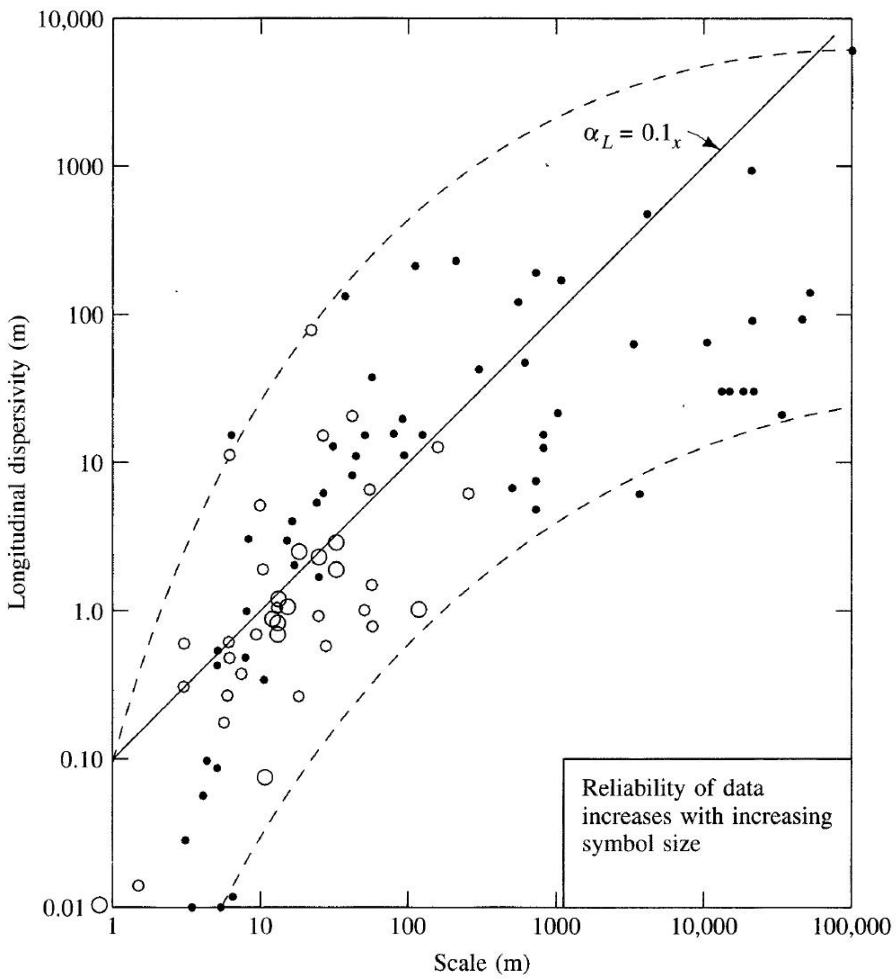
FIGURE 2.23 Field-measured values of longitudinal dispersivity as a function of the scale of measurement.



Source: P. Lallemand-Barres and P. Peaudecerf. 1978. *Bulletin, Bureau de Recherches Géologiques et Miniéres* 3/4: 277–284. Editions BRGM BP6009 45060 ORLEANS CEDEX 2.

Scale effects of dispersion

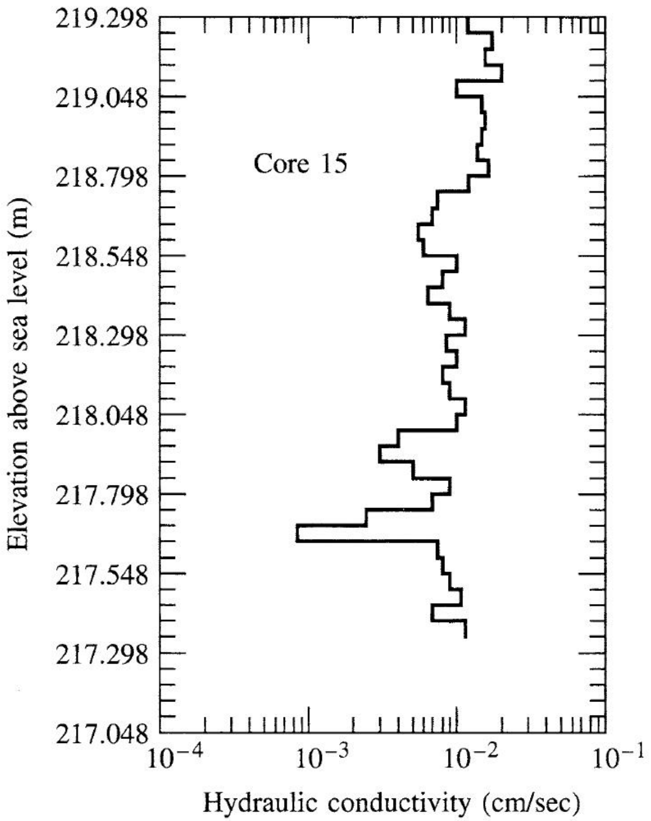
FIGURE 2.24 Field-measured values of longitudinal dispersivity as a function of the scale of measurement. The largest circles represent the most reliable data.



Source: L. W. Gelhar. 1986. Water Resources Research 22:135S–145S. Copyright by the American Geophysical Union. Reproduced with permission.

Scale effects of dispersion

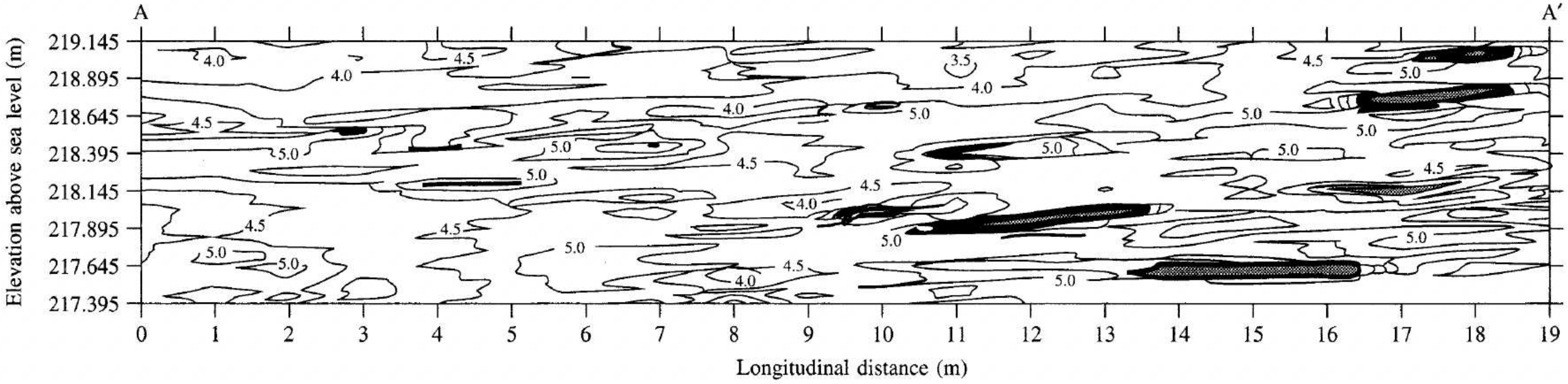
FIGURE 2.25 Hydraulic conductivity as determined by permeameter tests of remolded sediment samples from a glacial drift aquifer. The borings from which the cores were obtained are separated by one meter horizontally.



Source: E. A Sudicky, *Water Resources Research* 22, no. 13 (1986):2069–2082. Copyright by the American Geophysical Union. Reproduced with permission.

Scale effects of dispersion

FIGURE 2.26 Distribution of the hydraulic conductivity along a cross section through a glacial drift aquifer. Hydraulic conductivity is expressed as a negative log value. (If $K = 5 \times 10^{-2}$ cm/sec, then -log K is 1.3.) Sample locations are every 5 cm vertically and every 1 m horizontally. Hydraulic conductivity was less than 10^{-3} cm/sec in the stippled zones.



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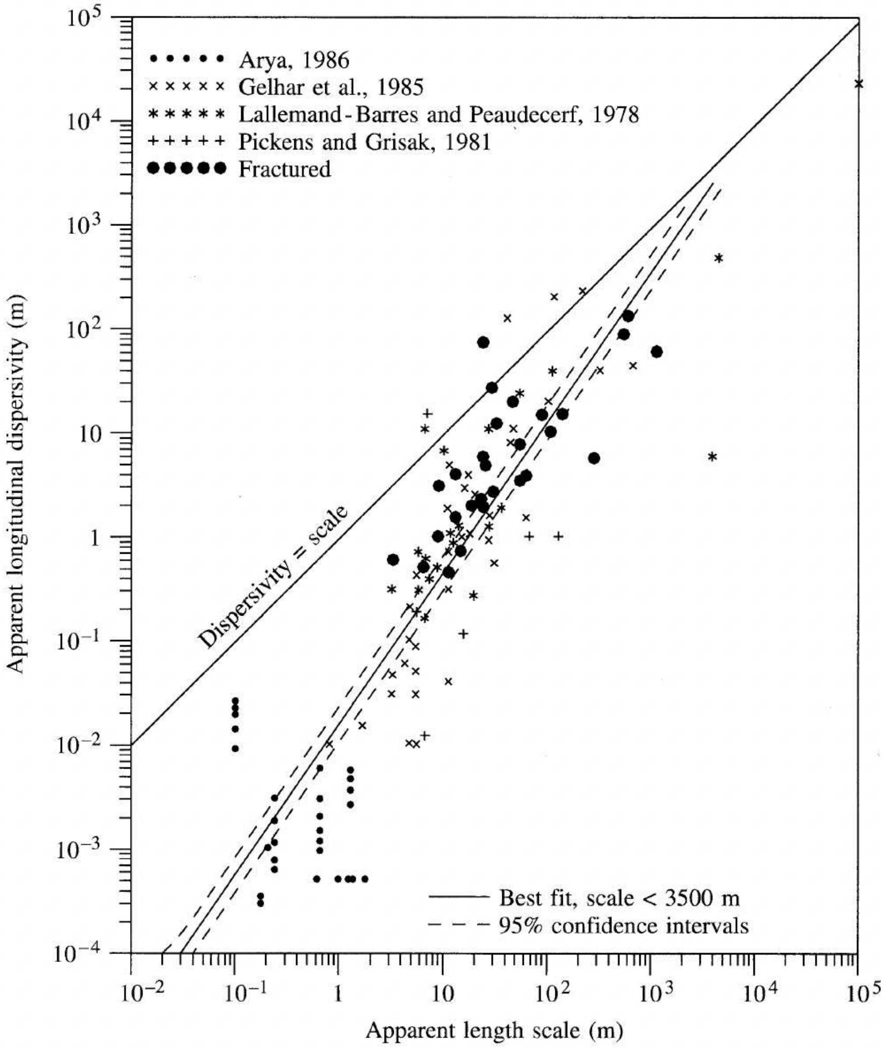
Scale effects of dispersion

FIGURE 2.28 Apparent longitudinal dispersivity from field and laboratory studies as a function of the scale of the study. Results from the calibration of numerical models are not included.



Correlation equation

$$\alpha_L = 0.0175L^{1.46}$$

Updated correlation equation (Xu and Eckstein,1995)

$$\alpha_L = 0.83(\log L)^{2.414}$$

Correction of Xu and Eckstein (1995) [Al-Suwaiyan, 1996]

$$\alpha_L = 0.82(\log L)^{2.446}$$

Source: S. Neuman. 1990. *Water Resources Research* 26:1749–1758. Copyright by the American Geophysical Union. Used with permission.