HWRS 561b
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Spring 2026

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)

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

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.

Non-dimensional form and dimensionless number

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)

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

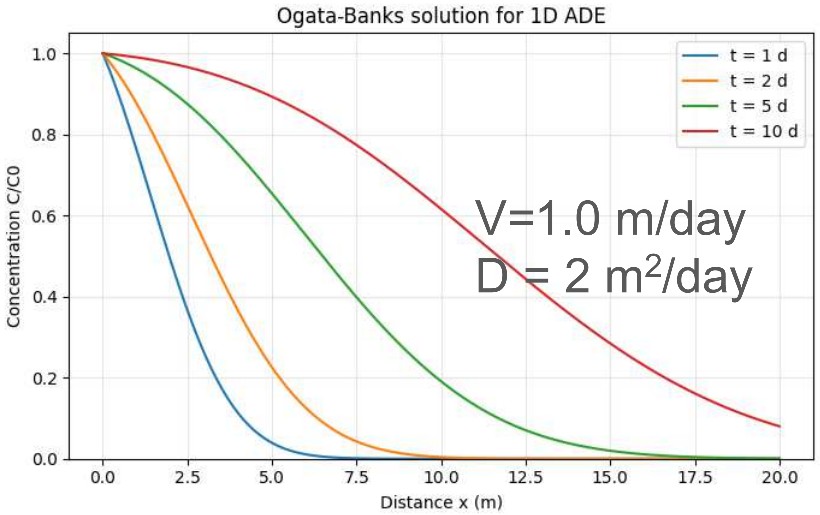
$$C(\infty,t) = 0,\ t \to \infty$$

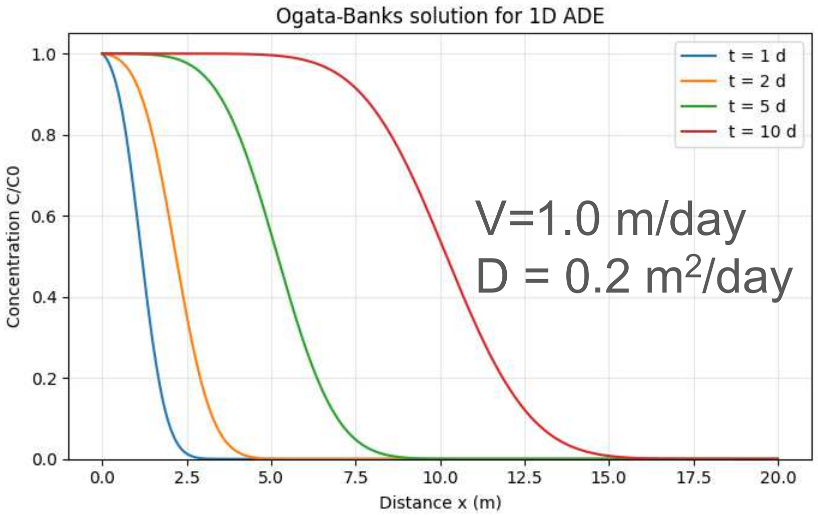
$$C = \frac{C_0}{2}\left[\mathrm{erfc}\left(\frac{x - Vt}{2\sqrt{Dt}}\right) + \exp\left(\frac{Vx}{D}\right)\mathrm{erfc}\left(\frac{x + Vt}{2\sqrt{Dt}}\right)\right]$$

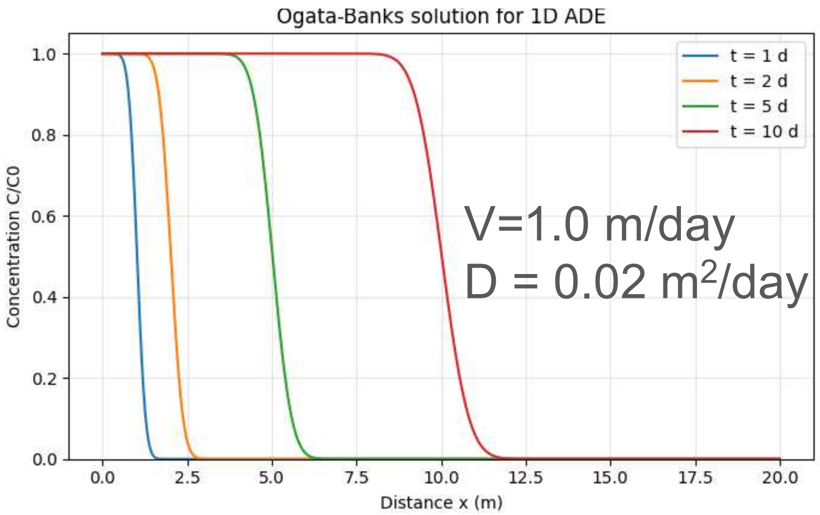
[Ogata and Banks, 1961]

1D step change in concentration

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







1D step change in concentration

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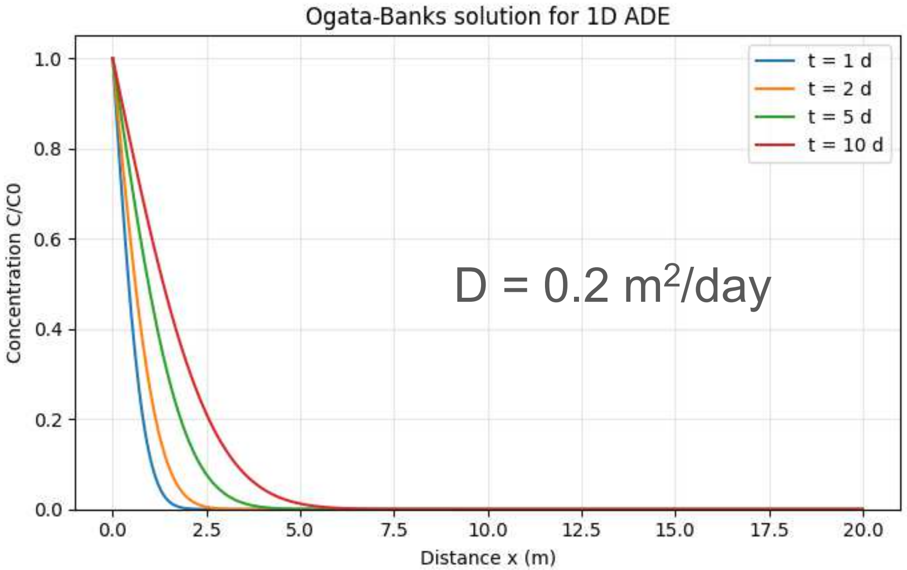
Gaussian distribution

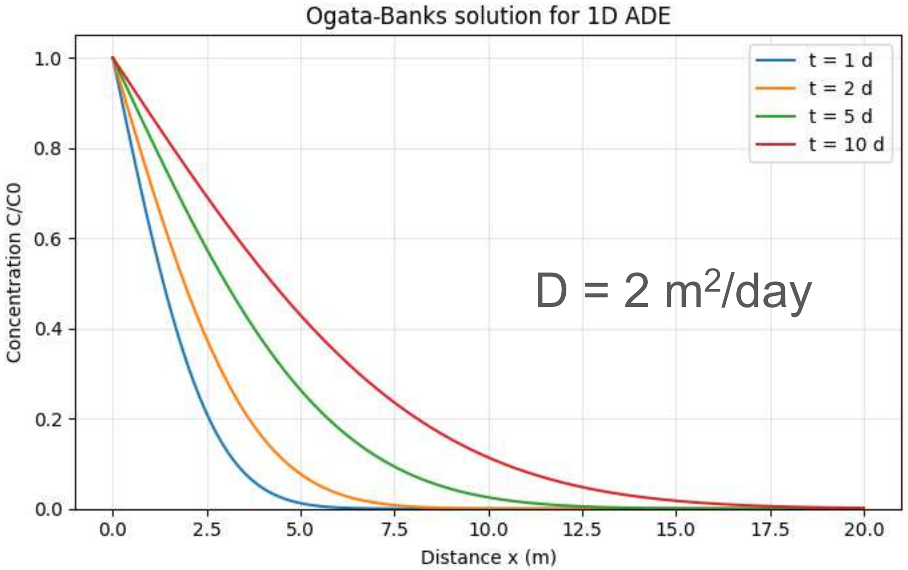
PDF $\frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$

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

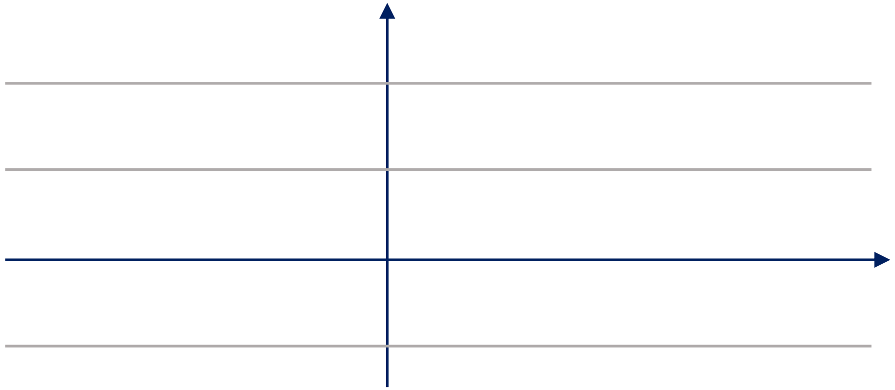
Special case: *V=0* (only dispersion)

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





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



1D step change in concentration

Characteristic time scales for advection and dispersion

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

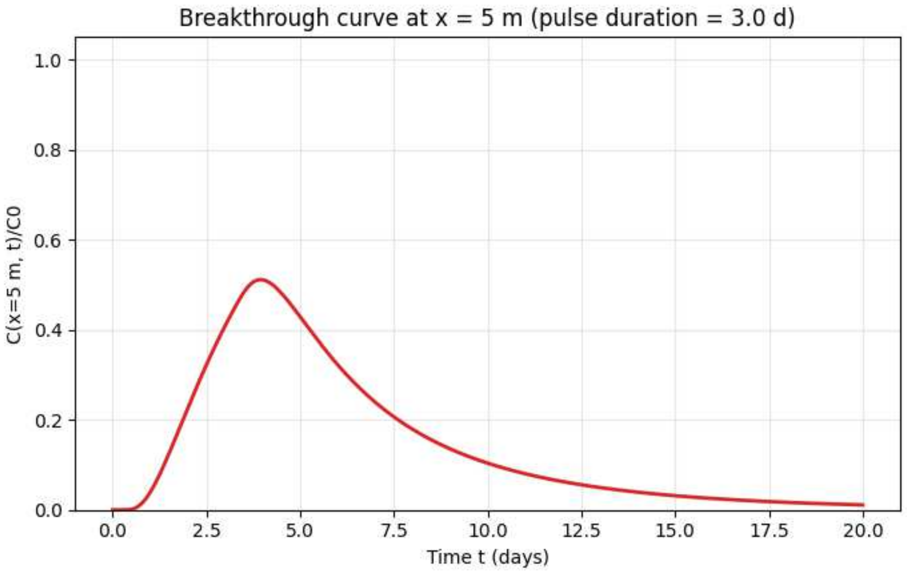
$0 \le t < t_0$

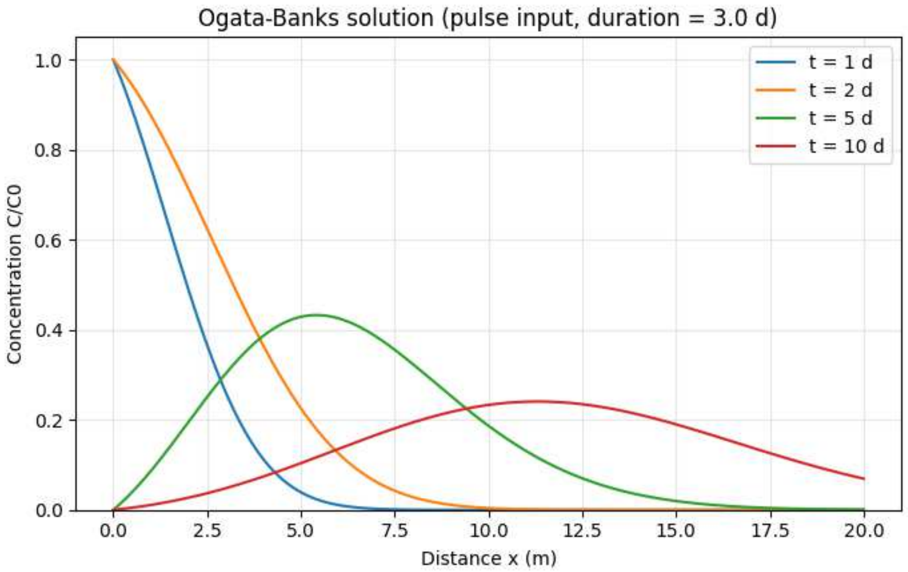
$$C = F(x,t)$$

$t \ge t_0$

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

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

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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.

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

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

Continuous injection (3rd-type boundary condition)

Initial condition

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

Boundary conditions (assuming semi-infinite domain)

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

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

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

[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.

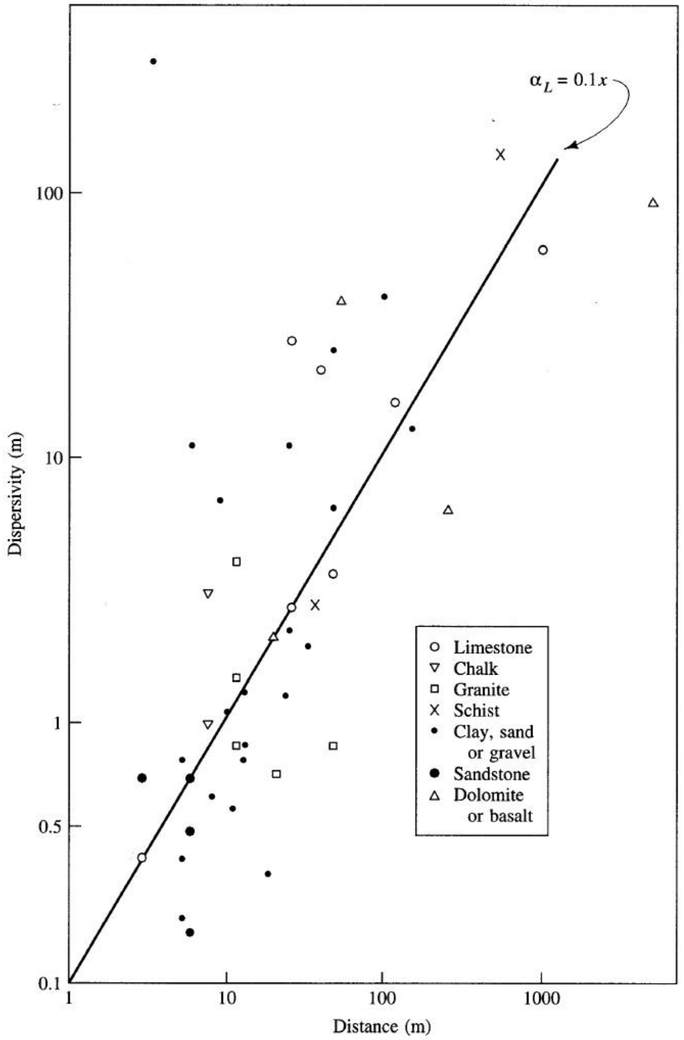
Substituting the solution for the volume-based concentration (from previous slide), we obtain the flux-based concentration

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

[van Genuchten, 1981]

Scale effects of dispersion

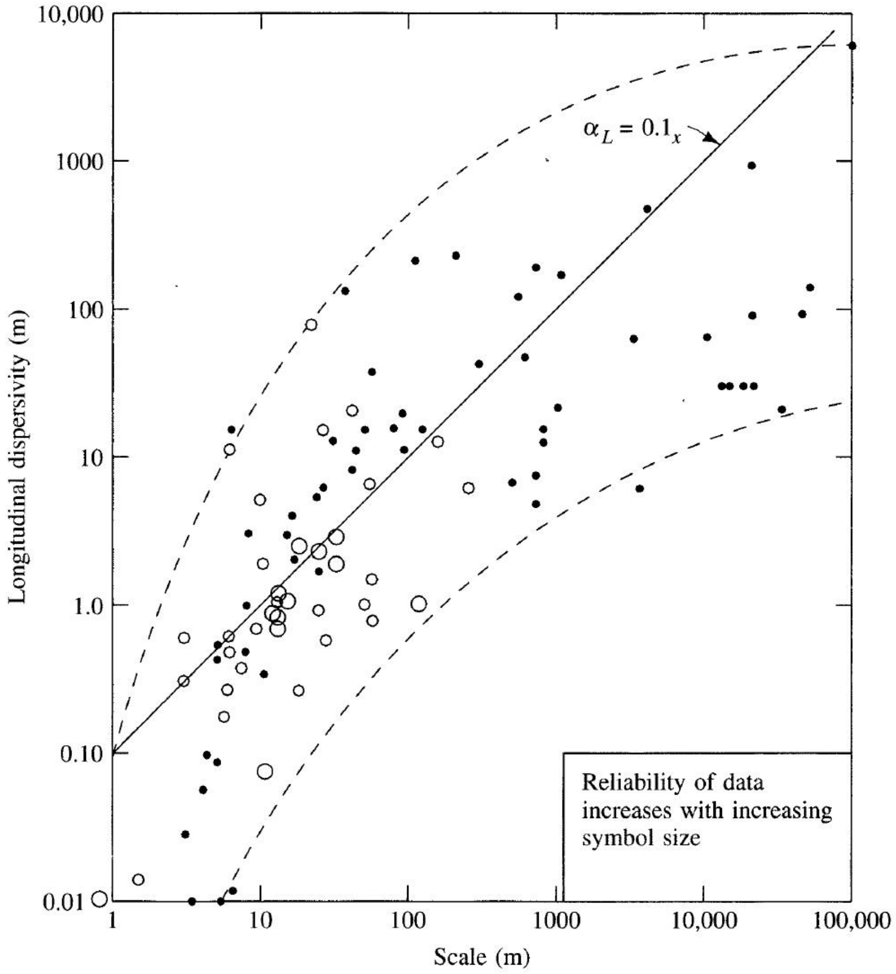
FIGURE 2.23 Field-measured values of longitudinal dispersivity as a function of the scale of measurement.



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.

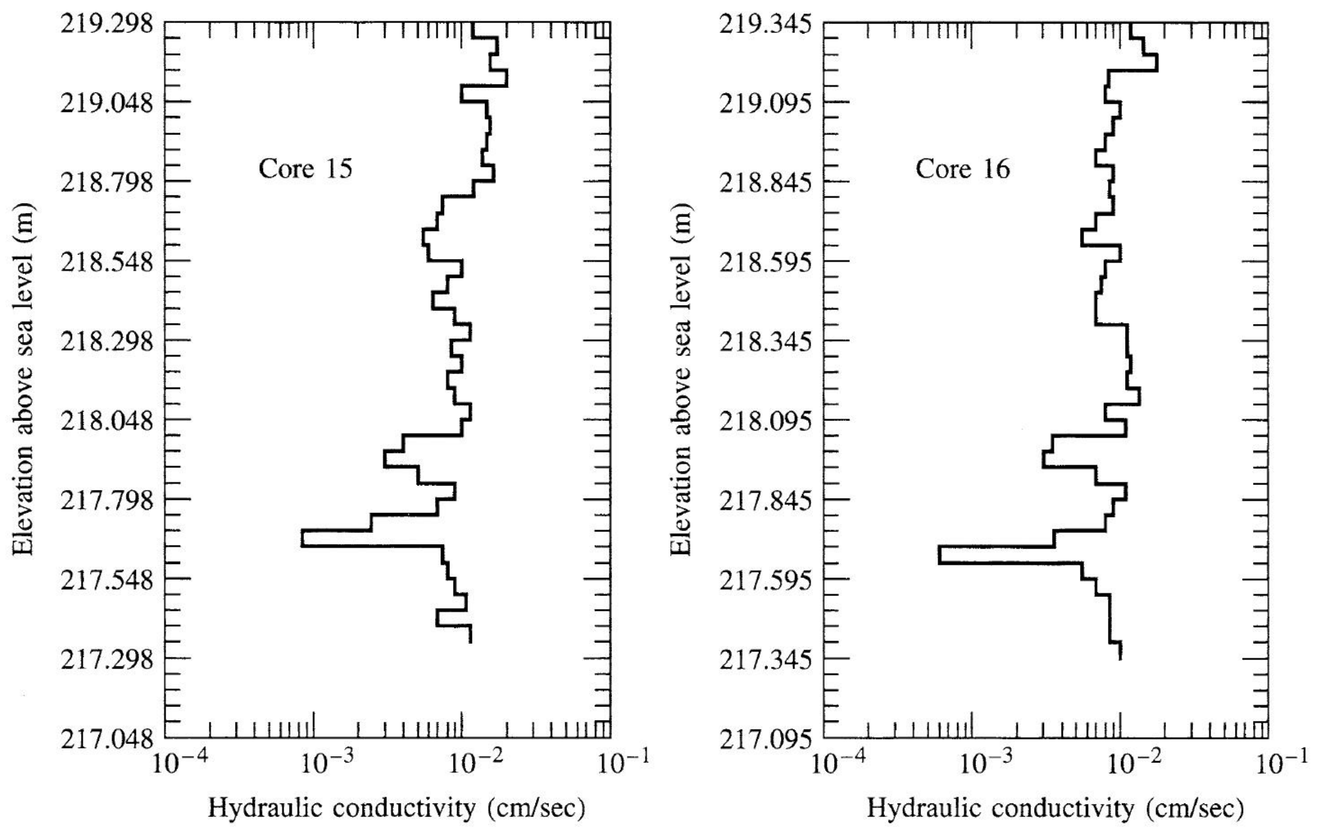
Scale effects of dispersion

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.



Scale effects of dispersion

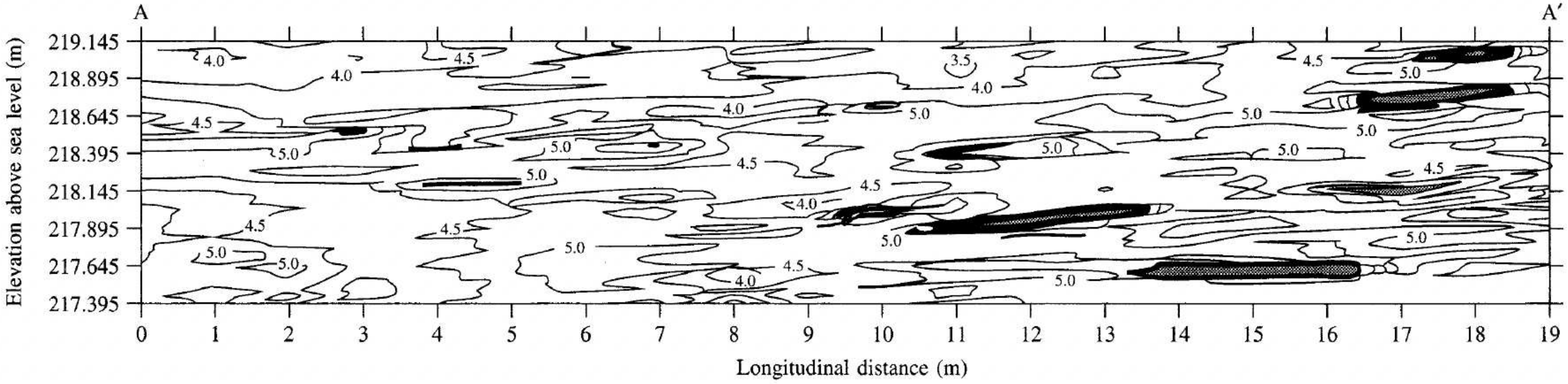
FIGURE 2.25 Hydraulic conductivity as determined by permeameter tests of remolded sediment samples from a glacial drift aquifer. The borings from which the cores were obtained are separated by one meter horizontally.



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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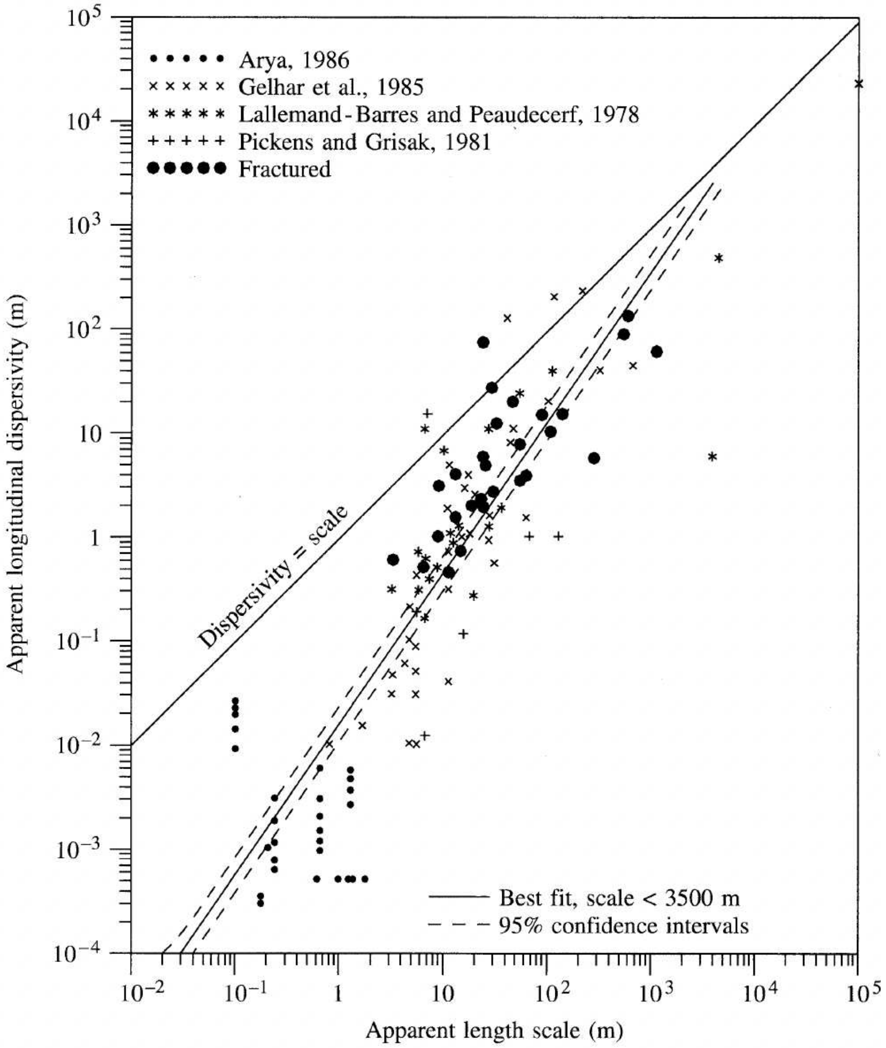
Scale effects of dispersion

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.



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

Correlation equation

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

Updated correlation equation (Xu and Eckstein,1995)

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

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

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