

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)

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

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

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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)

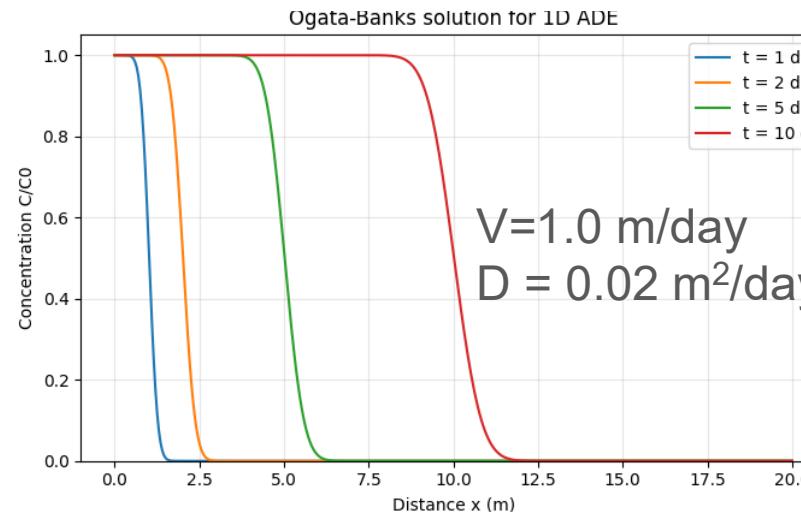
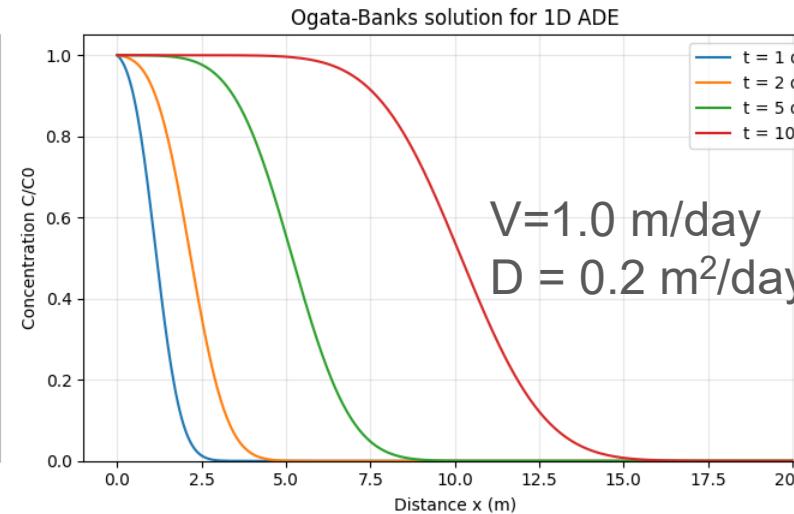
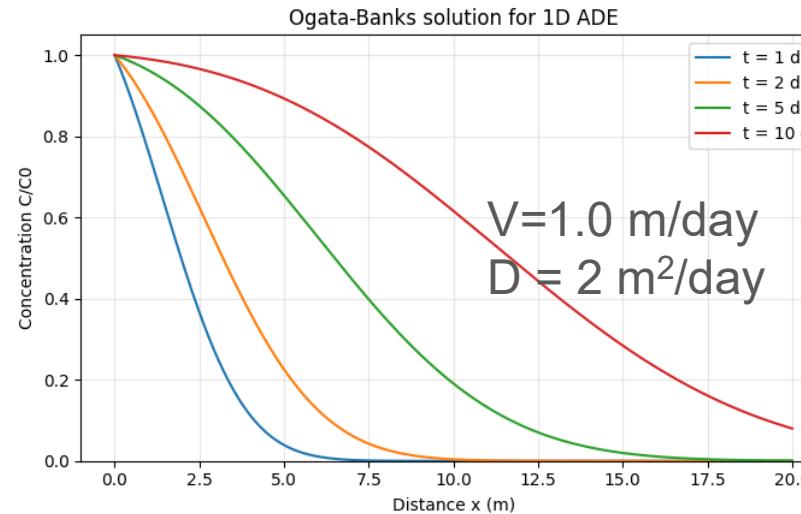
$$C(0, t) = C_0, t \geq 0$$

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

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

1D step change in concentration

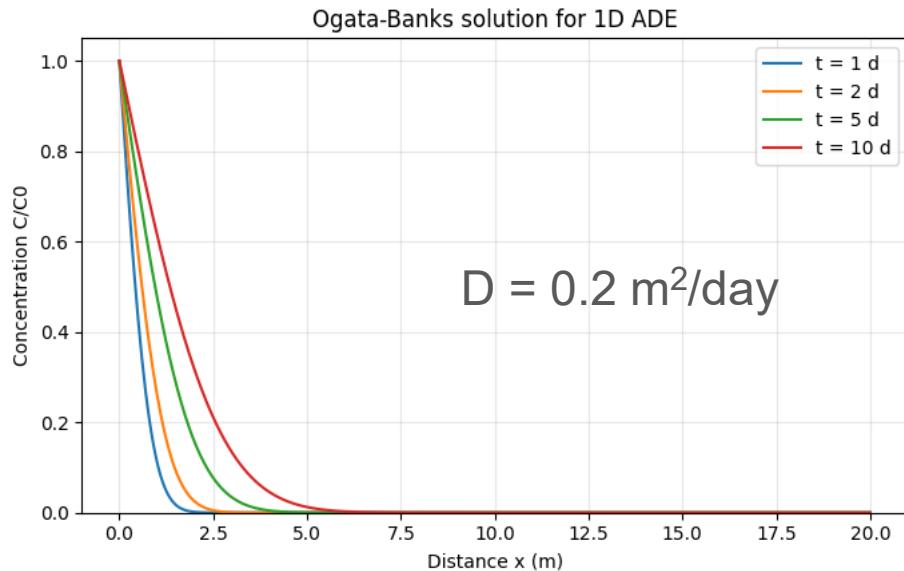
$$C = \frac{C_0}{2} \left[\operatorname{erfc} \left(\frac{x - Vt}{2\sqrt{Dt}} \right) + \exp \left(\frac{VL}{D} \right) \operatorname{erfc} \left(\frac{x + Vt}{2\sqrt{Dt}} \right) \right]$$



1D step change in concentration

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

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



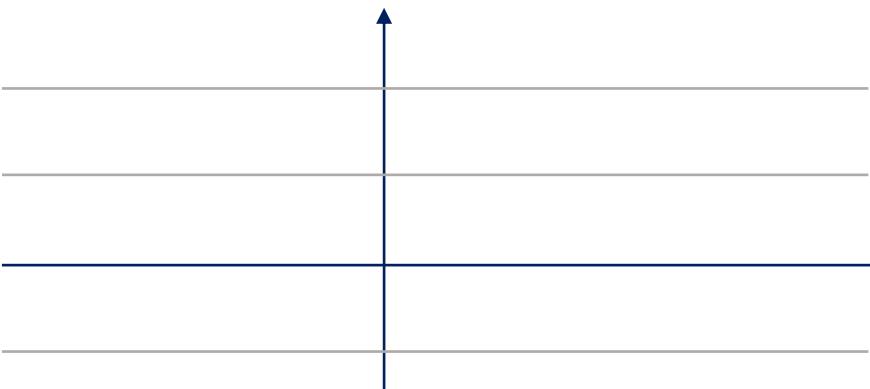
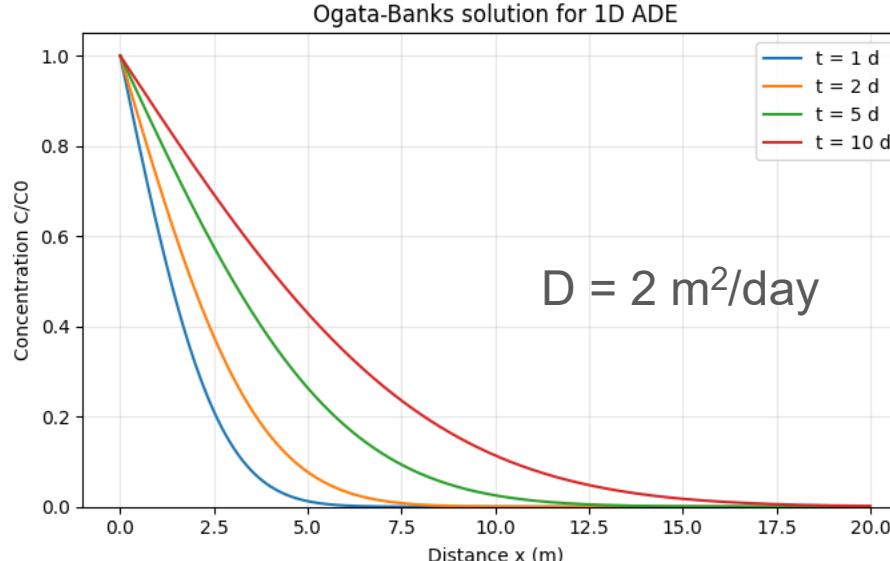
$$\operatorname{erfc}(x) = 1 - \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt = 1 - \operatorname{erf}(x)$$

Gaussian distribution

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

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

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1D step change in concentration

Characteristic time scales for advection and dispersion

1D pulse change in concentration

Pulse change in concentration

$$C(0, t) = C_0, \quad 0 \leq t \leq t_0$$

$$C(0, t) = 0, \quad t \geq t_0$$

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

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

Then, the solution for pulse change can be written as

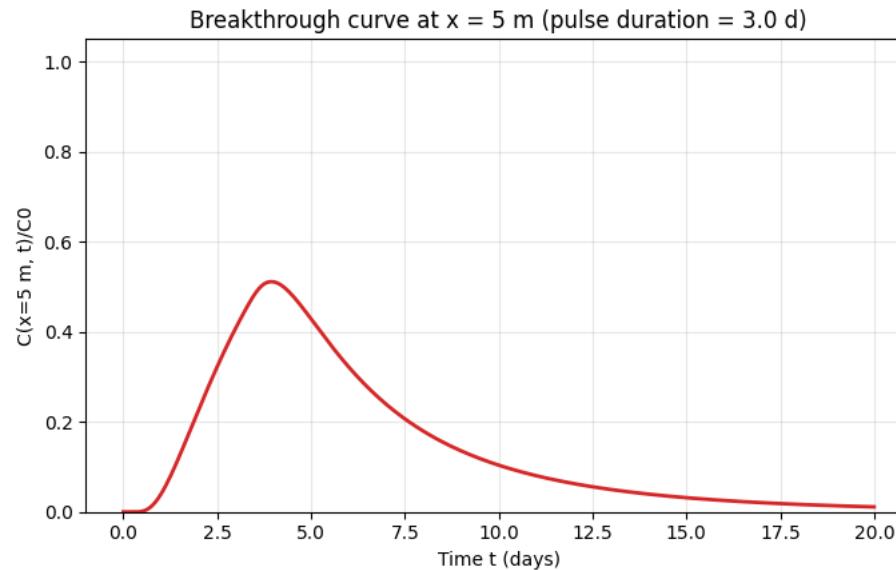
$$0 \leq t < t_0$$

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

$$t \geq t_0$$

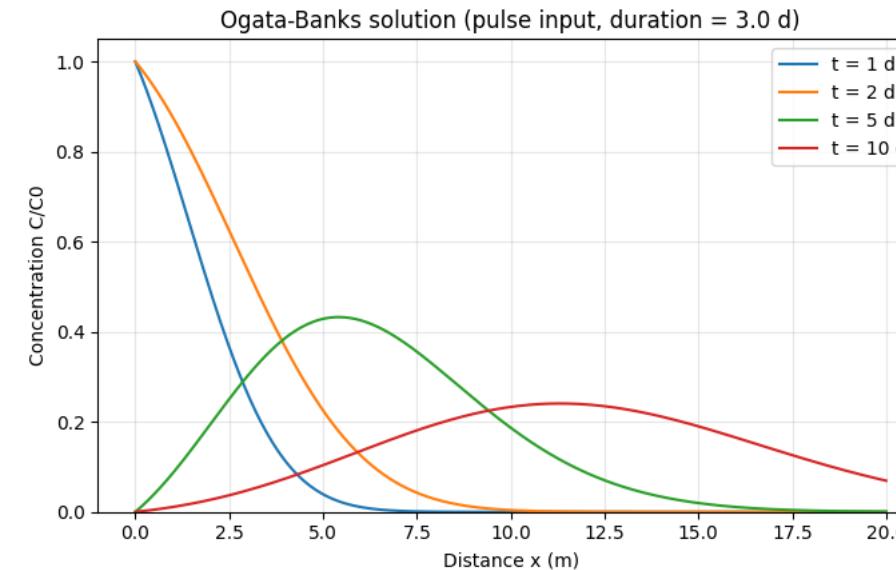
$$C = F(x, t) - F(x, t - t_0)$$

Moment analysis



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

Total mass passing the observation point.



Pulse injection

$$C(0, t) = C_0, 0 \leq t \leq t_0$$

$$C(0, t) = 0, t \geq t_0$$

$$t_0 = 3 \text{ d}$$

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

Arrival time

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

Travel time
(T_0 is the pulse duration)

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

Total mass in the system at a given 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

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

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

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

Continuous injection (3rd-type boundary condition)

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Initial condition

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

Boundary conditions (assuming semi-infinite domain)

$$\left. \left(-D \frac{\partial C}{\partial x} + V C \right) \right|_{x=0} = V C_0$$

$$\left. \frac{\partial C}{\partial x} \right|_{x \rightarrow \infty} = (\text{finite})$$

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

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).

$$\frac{\partial C}{\partial x} \Big|_{x=L} = 0$$

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

$$\left(-D \frac{\partial C}{\partial x} + V C \right) \Big|_{x=L} = V C_f \quad \text{where } C_f \text{ is the flux-based concentration as if there is no dispersive flux, i.e., all of the flux occurs as advection.}$$

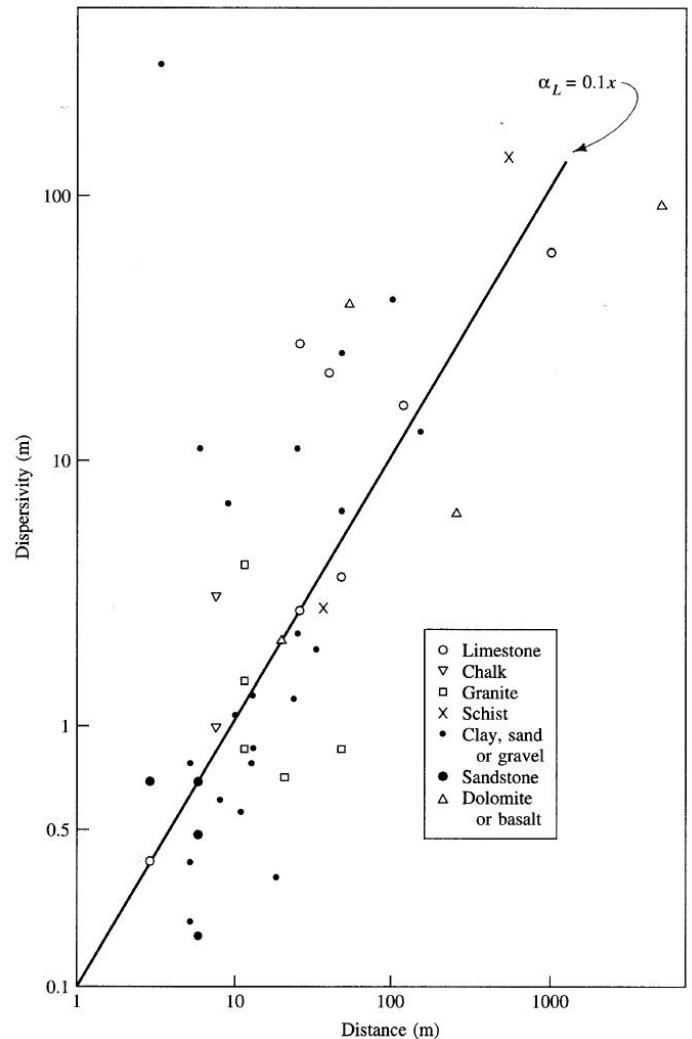
Substituting the solution for the volume-based concentration (from previous slide), we obtain the flux-based concentration

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

[van Genuchten, 1981]

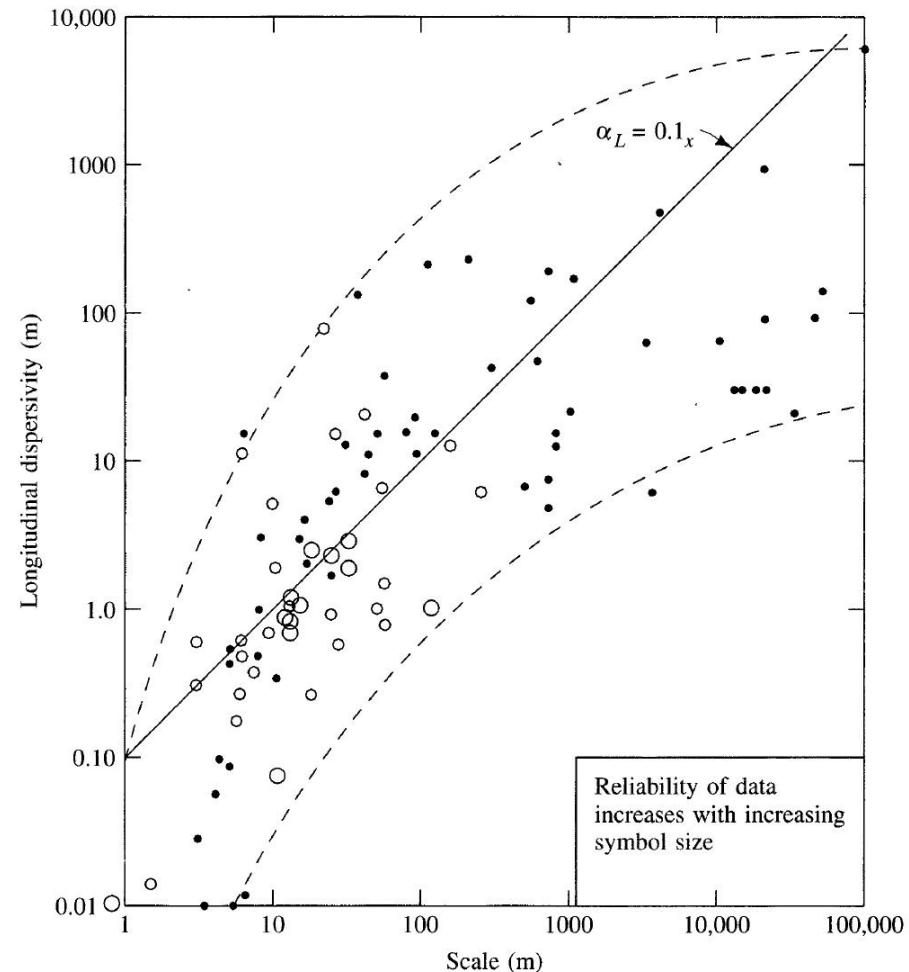
Scale effects of dispersion

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



Scale effects of dispersion

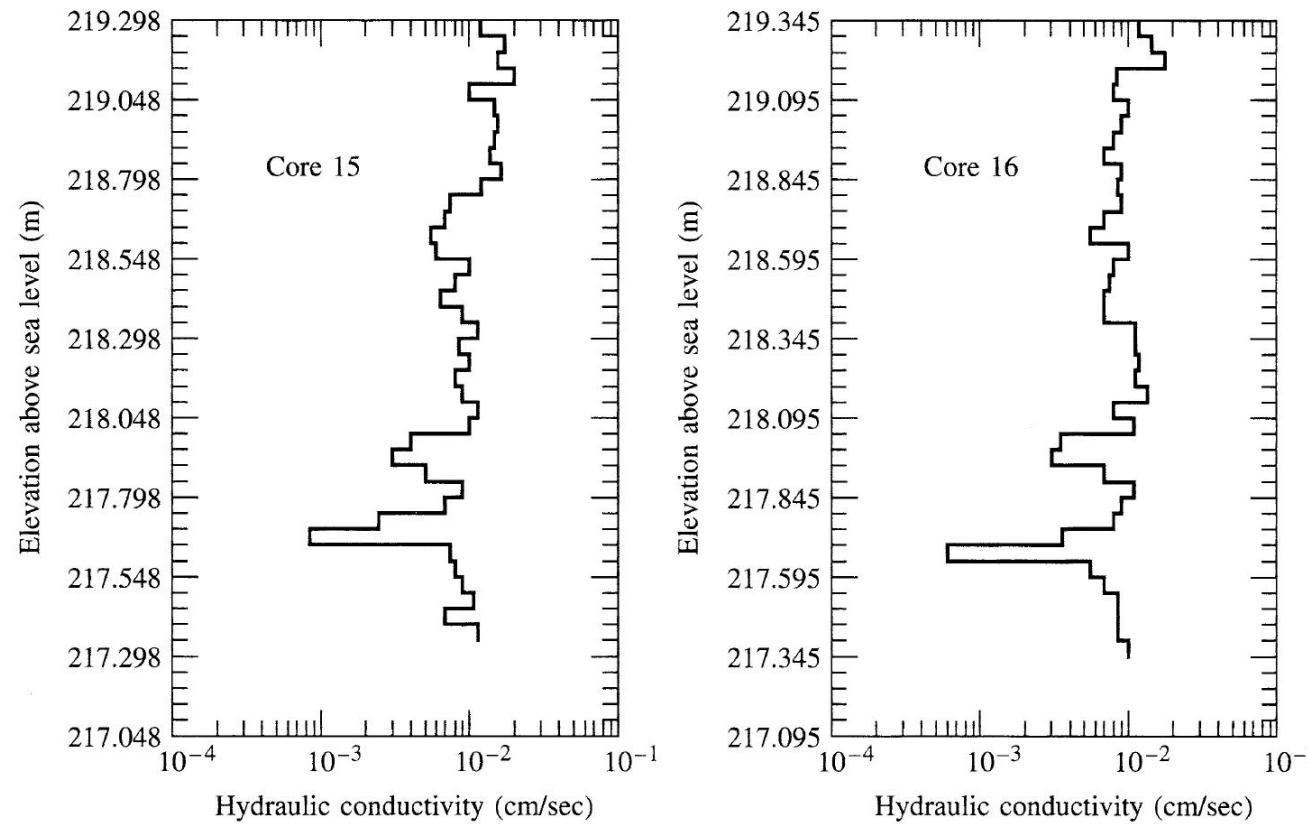
FIGURE 2.24 Field-measured values of longitudinal dispersivity as a function of the scale of measurement. The largest circles represent the most reliable data.



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Scale effects of dispersion

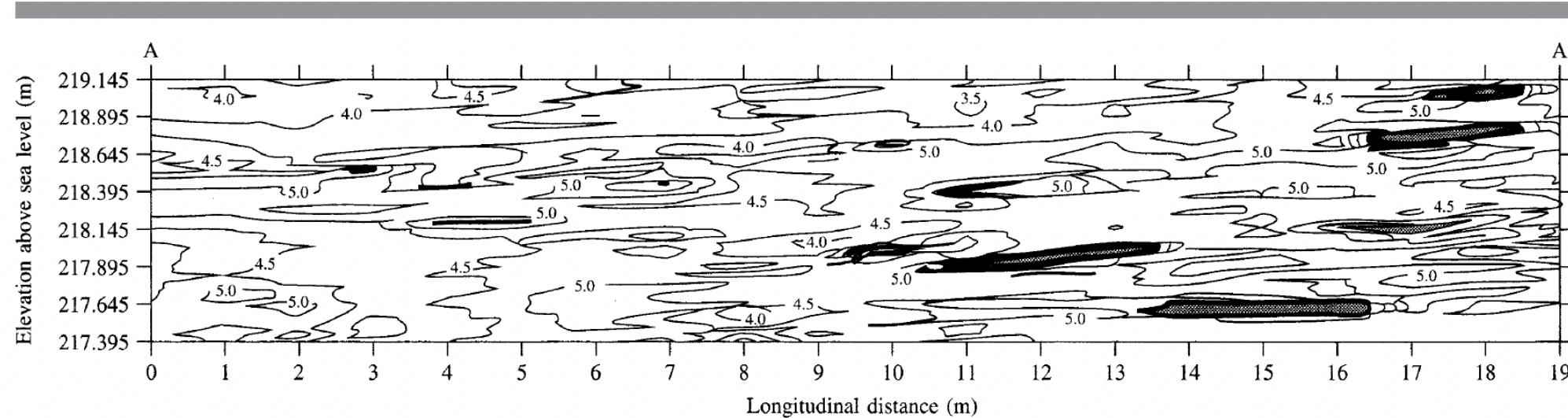
FIGURE 2.25 Hydraulic conductivity as determined by permeameter tests of remolded sediment samples from a glacial drift aquifer. The borings from which the cores were obtained are separated by one meter horizontally.



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

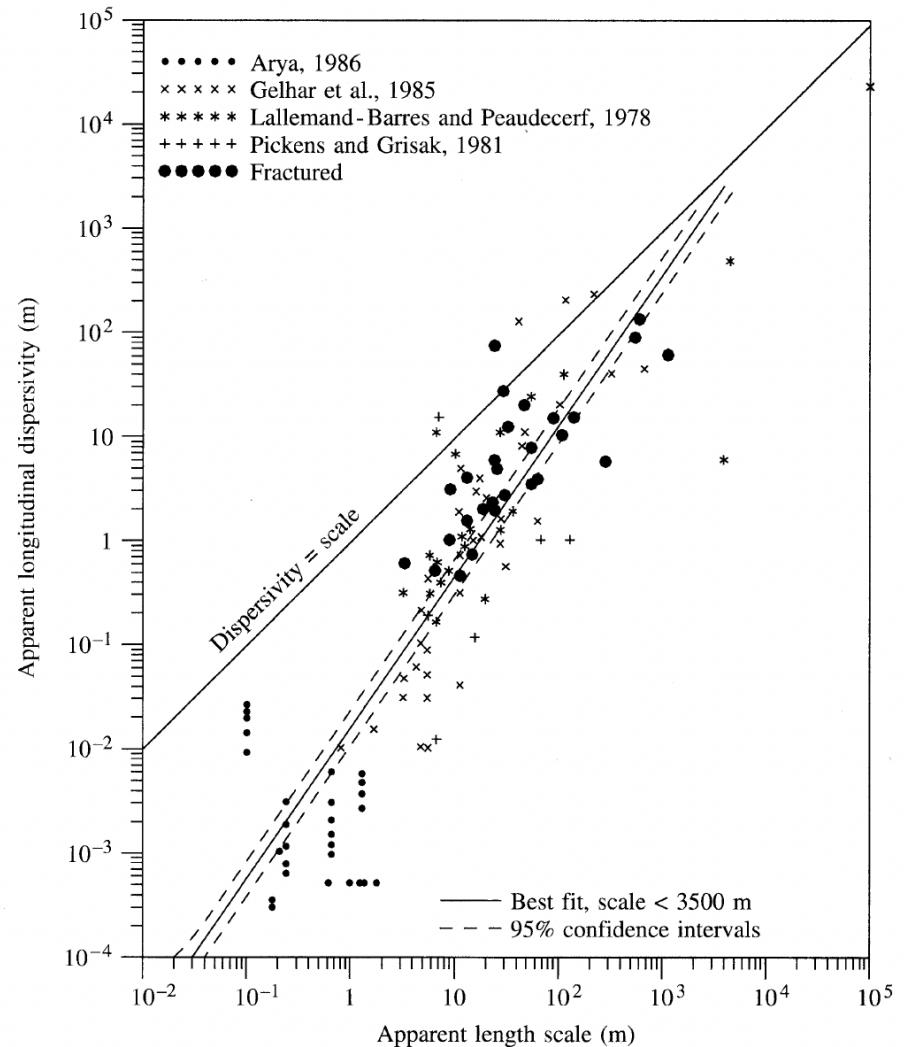
FIGURE 2.26 Distribution of the hydraulic conductivity along a cross section through a glacial drift aquifer. Hydraulic conductivity is expressed as a negative log value. (If $K = 5 \times 10^{-2}$ cm/sec, then $-\log K$ is 1.3.) Sample locations are every 5 cm vertically and every 1 m horizontally.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

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