

# 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)

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

1)  $D \div \phi$   
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

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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:

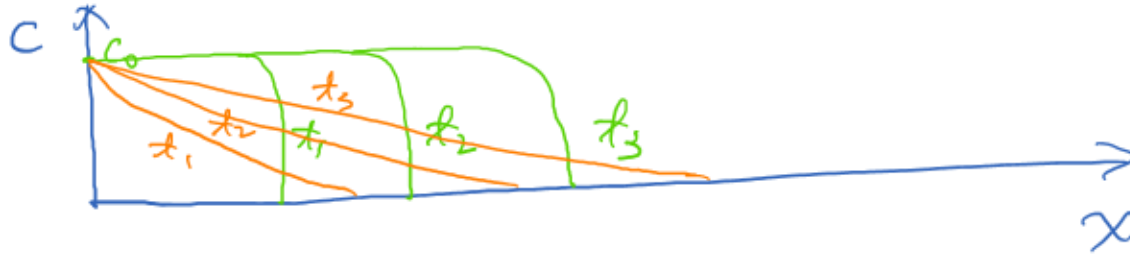
$$Pe = \frac{\text{Advective transport rate}}{\text{Dispersive transport rate}} = \frac{\text{Dispersive time scale}}{\text{Advective time scale}}$$

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

- 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)

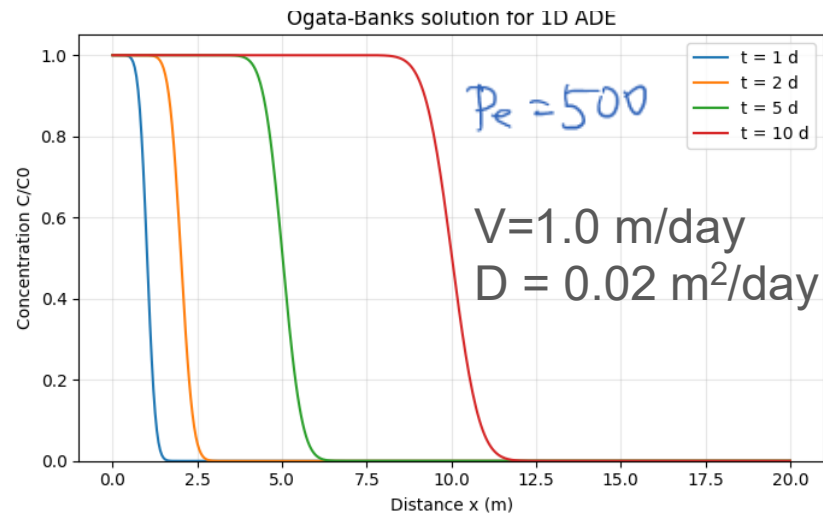
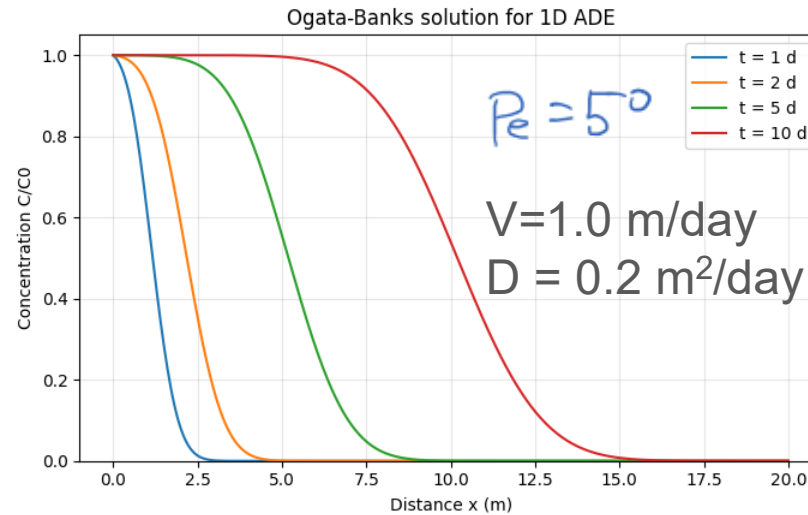
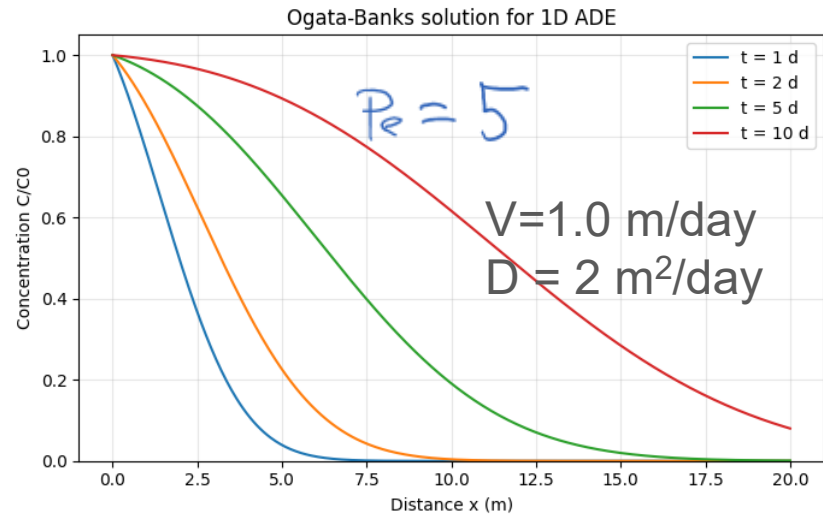
$$C(0, t) = C_0, t \geq 0$$

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

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

# 1D step change in concentration

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



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

$L = 10$

# 1D step change in concentration

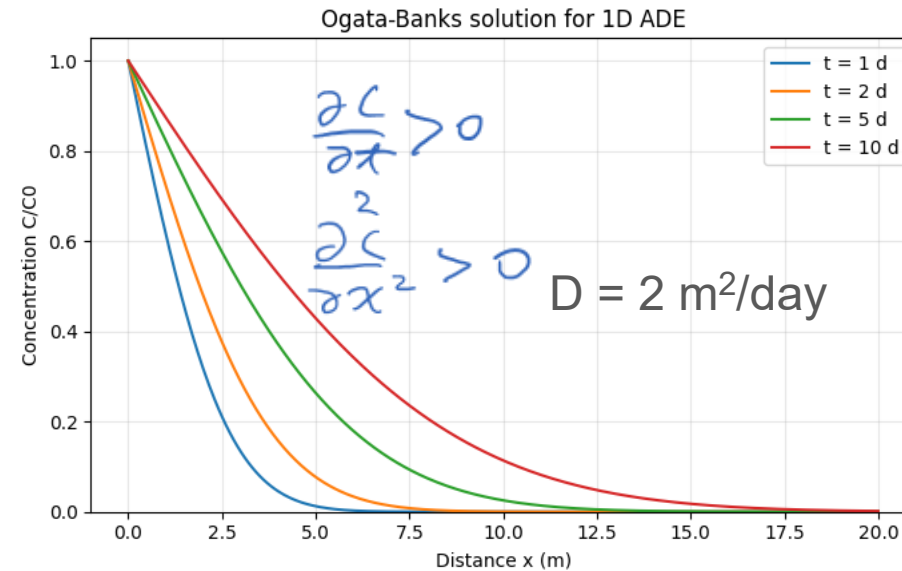
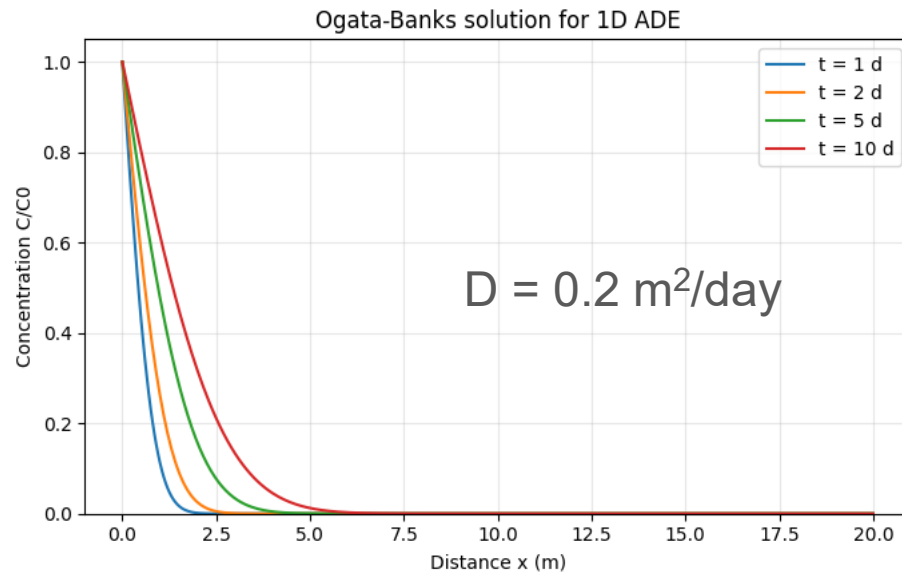
Special case:  $V=0$  (only dispersion)

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

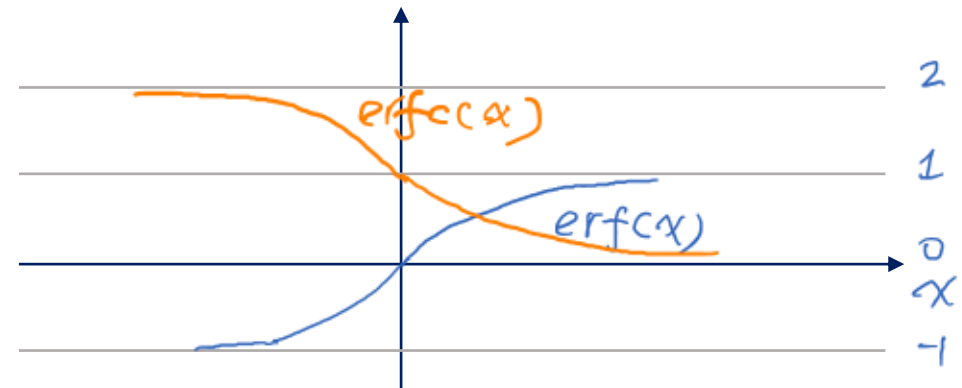
$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

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

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



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



# 1D step change in concentration

Characteristic time scales for advection and dispersion

Advection Equation:

$$\frac{\partial C}{\partial t} = -V \frac{\partial C}{\partial x}$$

Scaling analysis

$$C \sim C_0, t \sim \tau_c, x \sim x_c$$

$$\Rightarrow \frac{C_0}{\tau_c} \sim V \frac{C_0}{x_c}$$

$$\Rightarrow \tau_c \sim \frac{x_c}{V} = \frac{L}{V}$$

$$[\text{let } L = x_c]$$

Dispersion Equation:  
(Diffusion)

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

$$\frac{C_0}{\tau_c} \sim D \frac{C_0}{x_c^2} \Rightarrow \tau_c \sim \frac{x_c^2}{D} = \frac{L^2}{D}$$

"Baking turkey"



Heating is governed by

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

$\alpha$  heat conductivity

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

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

"Turkey twice big requires four times baking time!"



# 1D pulse change in concentration

Pulse change in concentration

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

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



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

$$0 \leq t < t_0$$

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

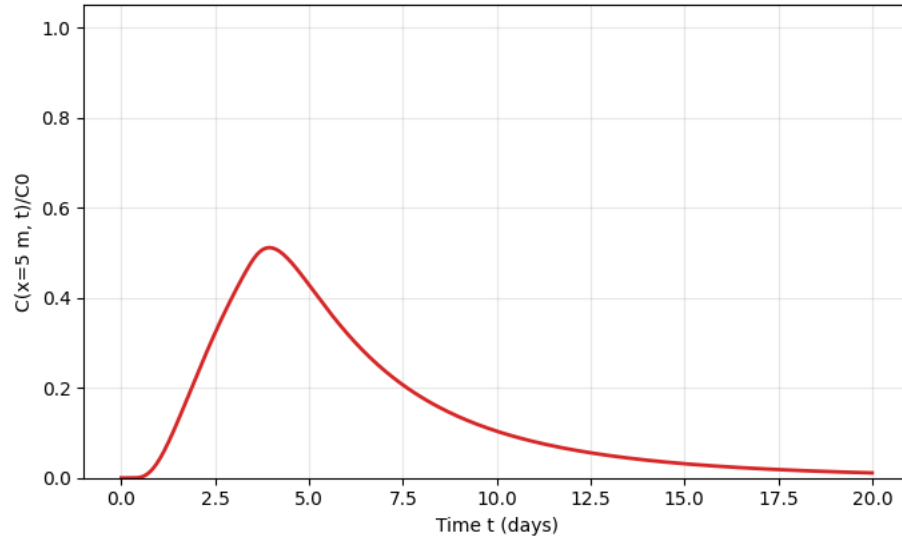
$$t \geq t_0$$

$$C = F(x, t) - \underbrace{F(x, t - t_0)}$$

subtract the solution for step change starting at  $t_0$ .

# Moment analysis

Breakthrough curve at  $x = 5$  m (pulse duration = 3.0 d)

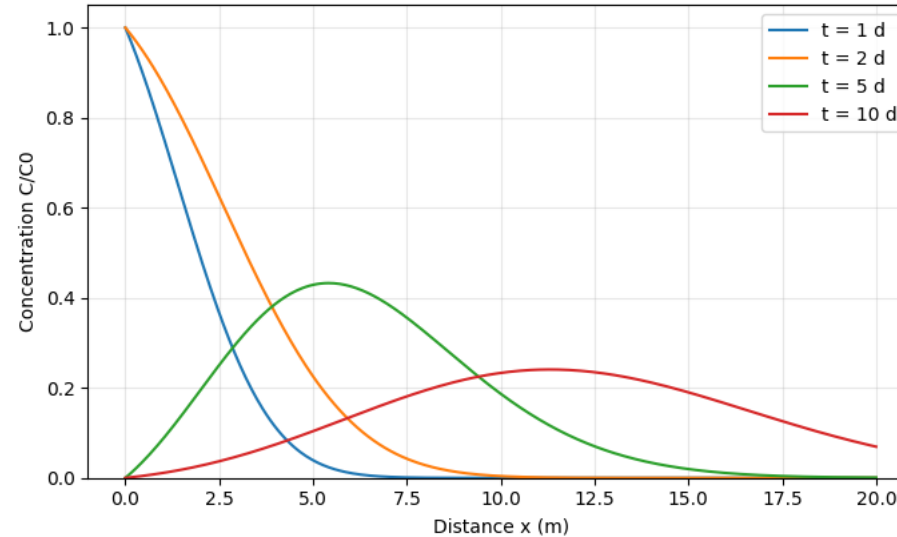


$$M_t^0 = \int_0^\infty C dt \quad \text{Total mass passing the observation point.}$$

$$M_t^1 = \frac{\int_0^\infty C t dt}{\int_0^\infty C dt} = \frac{\int_0^\infty C t dt}{M_t^0} \quad \text{Arrival time}$$

$$M_{t,adj}^1 = \frac{\int_0^\infty C t dt}{M_t^0} - \frac{1}{2}T_0 \quad \text{Travel time (} T_0 \text{ is the pulse duration)}$$

Ogata-Banks solution (pulse input, duration = 3.0 d)



$$M_s^0 = \int_0^\infty C dx \quad \text{Total mass in the system at a given time.}$$

$$M_x^1 = \frac{\int_0^\infty C x dx}{\int_0^\infty C dx} = \frac{\int_0^\infty C t dx}{M_x^0} \quad \text{Center of mass}$$

Pulse injection

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

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

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

# 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	$M_t^1 = \frac{\int_0^{\infty} Ct \, dt}{\int_0^{\infty} C \, dt} = \frac{\int_0^{\infty} Ct \, dt}{M_t^0}$	Arrival 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
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)	Not defined	
Second Central Moment	$M_t^2 = \frac{\int_0^{\infty} (t - M_t^1)^2 C \, dt}{M_t^0}$	Temporal variance	$M_s^2 = \frac{\int_0^{\infty} (x - M_s^1)^2 C \, dx}{M_s^0}$	Spatial 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	$M_s^3 = \frac{\int_0^{\infty} (x - M_s^1)^3 C \, dx}{M_s^0}$	Plume asymmetry in space
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	$M_s^4 = \frac{\int_0^{\infty} (x - M_s^1)^4 C \, dx}{M_s^0}$	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.

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

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

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

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

# Continuous injection (3<sup>rd</sup>-type boundary condition)

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Initial condition

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

Boundary conditions (assuming semi-infinite domain)

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

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

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

# Continuous injection (3<sup>rd</sup>-type boundary condition)

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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

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

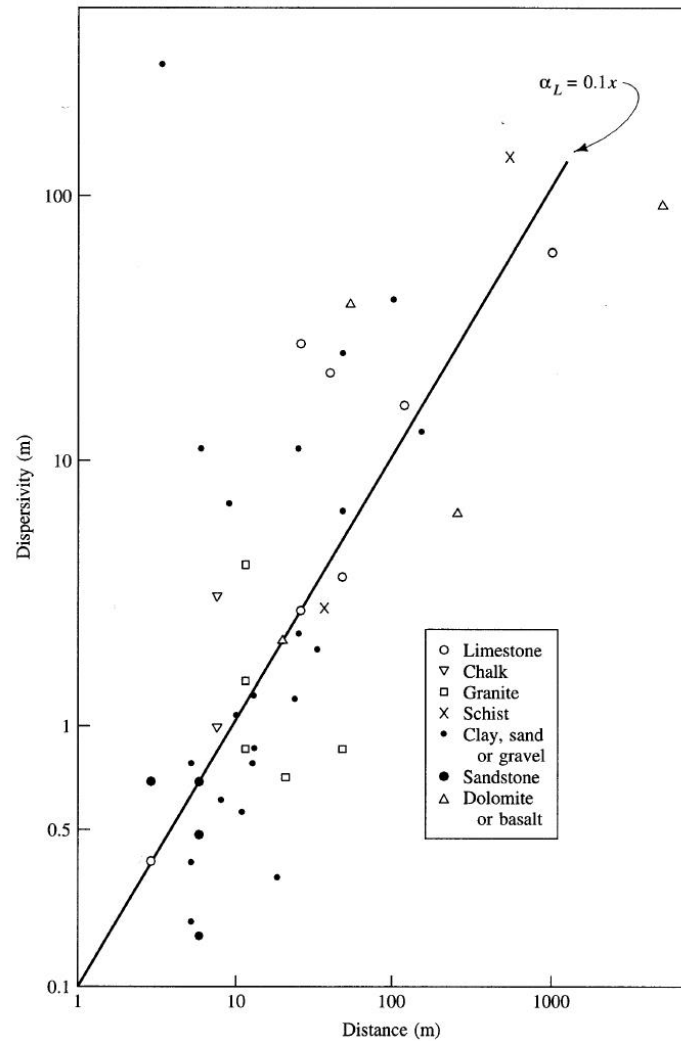
Substituting the solution for the volume-based concentration (from previous slide), we obtain the flux-based concentration

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

[van Genuchten, 1981]

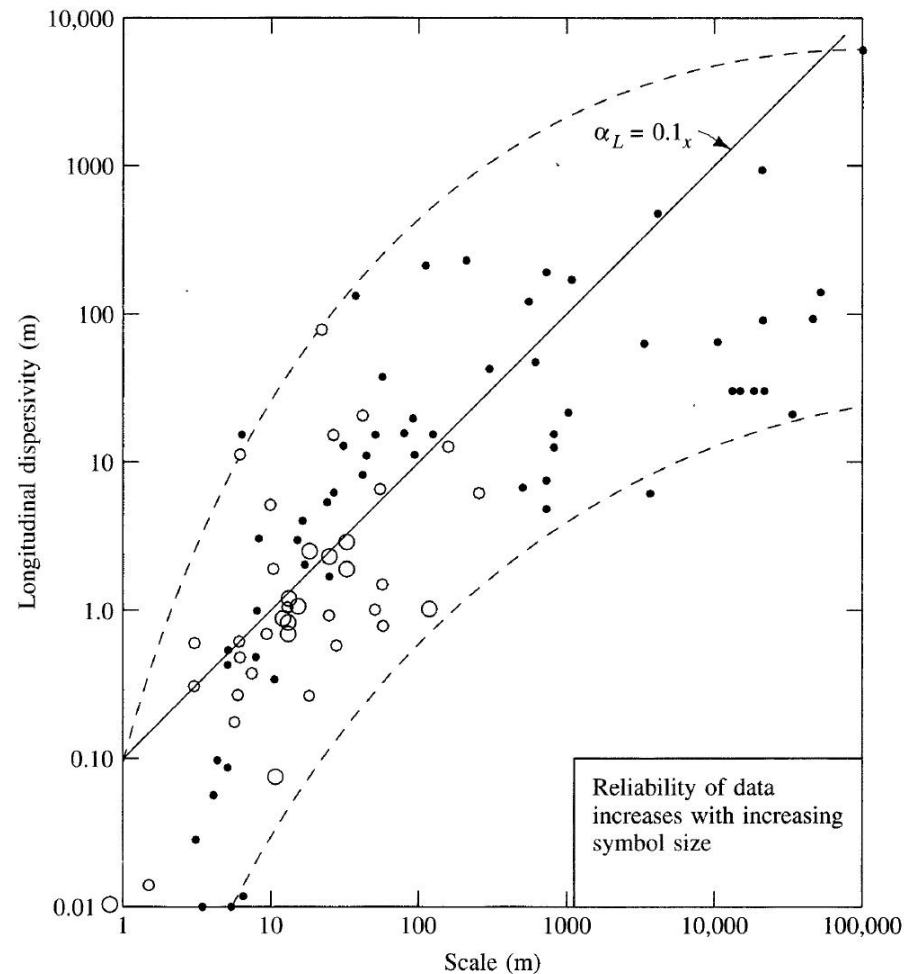
# Scale effects of dispersion

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



# Scale effects of dispersion

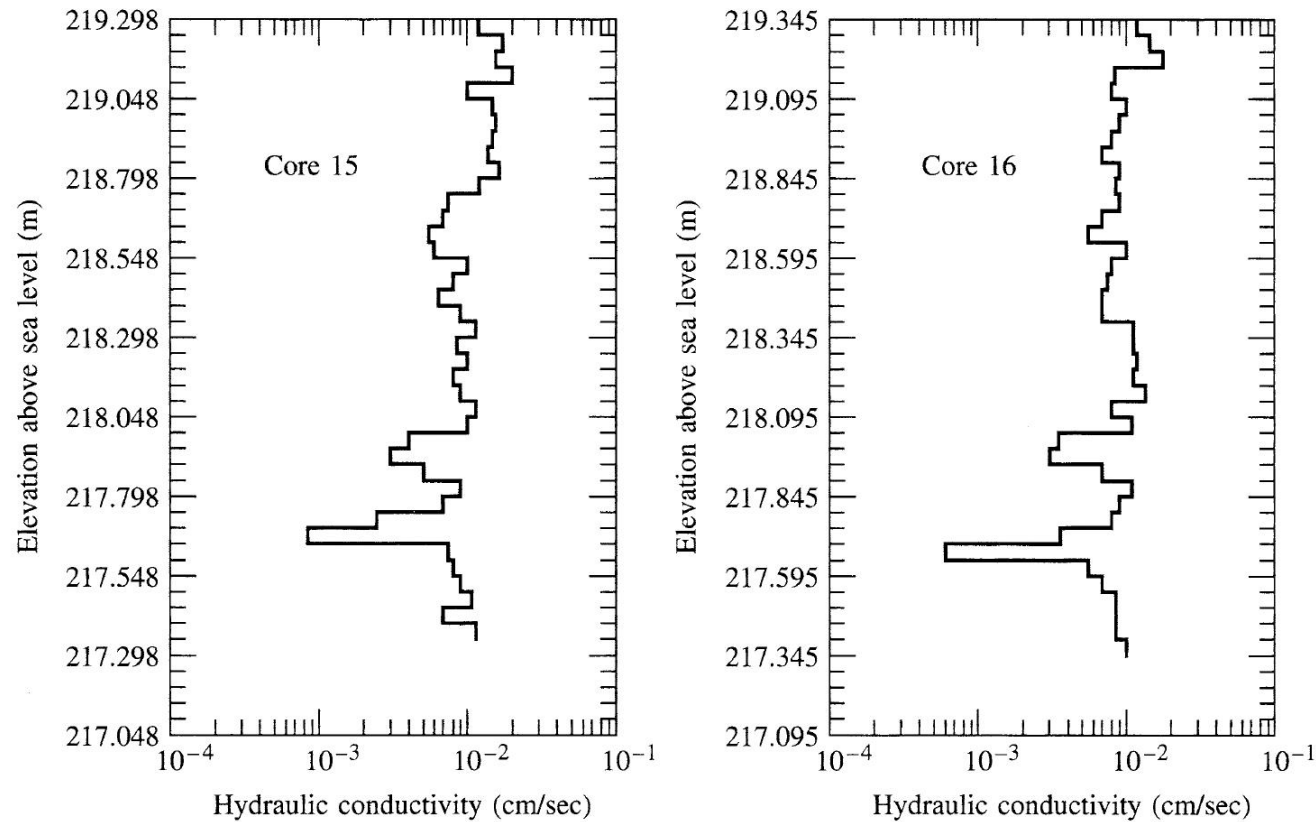
**FIGURE 2.24** Field-measured values of longitudinal dispersivity as a function of the scale of measurement. The largest circles represent the most reliable data.





# Scale effects of dispersion

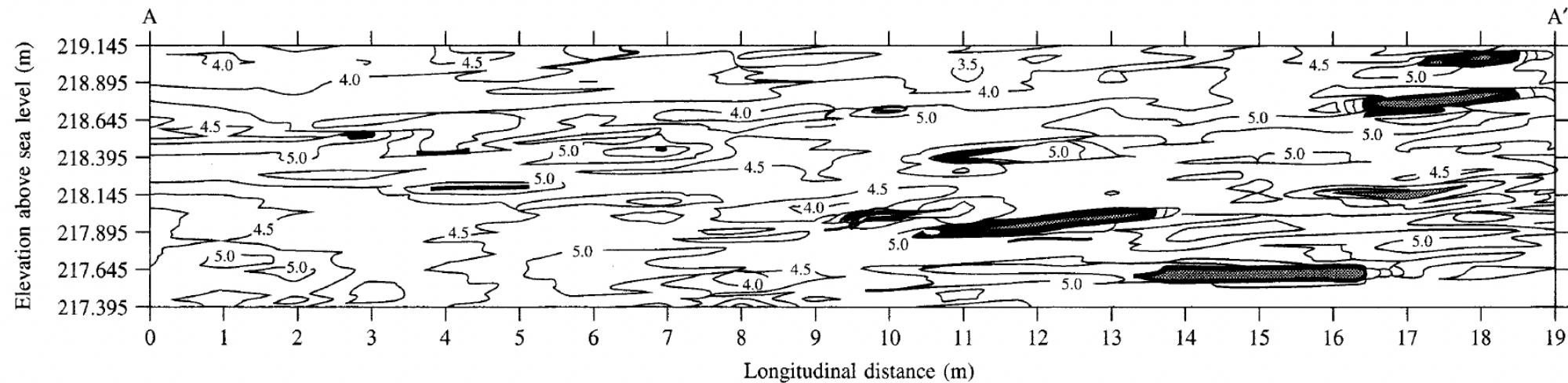
**FIGURE 2.25** Hydraulic conductivity as determined by permeameter tests of remolded sediment samples from a glacial drift aquifer. The borings from which the cores were obtained are separated by one meter horizontally.



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

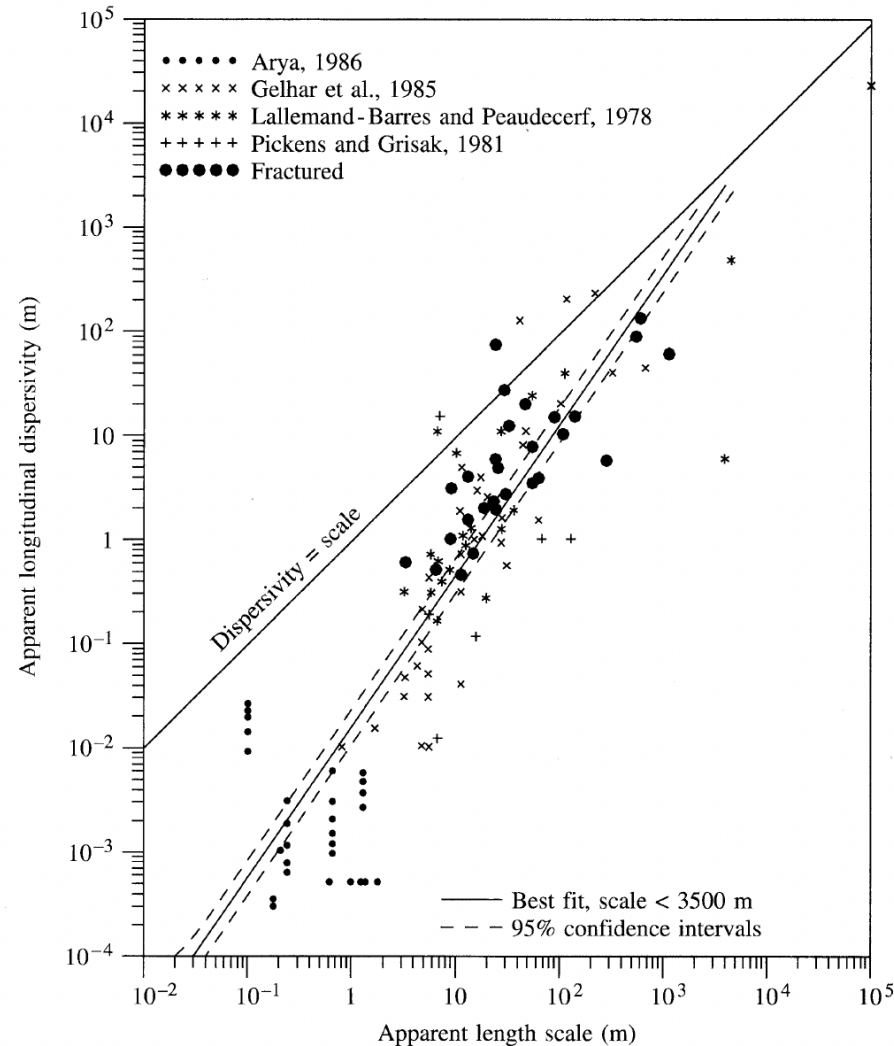
**FIGURE 2.26** Distribution of the hydraulic conductivity along a cross section through a glacial drift aquifer. Hydraulic conductivity is expressed as a negative log value. (If  $K = 5 \times 10^{-2}$  cm/sec, then  $-\log K$  is 1.3.) Sample locations are every 5 cm vertically and every 1 m horizontally.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



Source: E. A Sudicky. 1986. *Water Resources Research* 22:2069–2082. Copyright by the American Geophysical Union. Reproduced with permission.

# 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]

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