

# HWRS 561b: Physical Hydrogeology II

## Solute transport (Part 3)

Agenda:

1. Analytical solutions for solute transport

# 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)

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

$\stackrel{1) \div \phi}{\cancel{D}}$   
 $\stackrel{2) V = v_x}{\cancel{V}}$   
 $\stackrel{3) D = D_{xx}}{\cancel{D}}$

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  $\tilde{x} = \frac{x}{L}$ ,  $\tilde{t} = \frac{t}{LV}$ ,  $\tilde{c} = \frac{c}{c_0}$

$$\frac{\partial c}{\partial t} = \frac{\partial (\tilde{c} c_0)}{\partial (\tilde{t} LV)} = \frac{V c_0}{L} \frac{\partial \tilde{c}}{\partial \tilde{t}}$$

$$V \frac{\partial c}{\partial x} = V \frac{\partial (\tilde{c} c_0)}{\partial (\tilde{x} L)} = \frac{V c_0}{L} \frac{\partial \tilde{c}}{\partial \tilde{x}}$$

$$D \frac{\partial^2 c}{\partial x^2} = D \frac{\partial^2 (\tilde{c} c_0)}{\partial (\tilde{x} L)^2} = \frac{D c_0}{L^2} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}^2}$$

$$\frac{V c_0}{L} \frac{\partial \tilde{c}}{\partial \tilde{t}} + \frac{V c_0}{L} \frac{\partial \tilde{c}}{\partial \tilde{x}} - \frac{D c_0}{L^2} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}^2} = 0$$

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

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 :

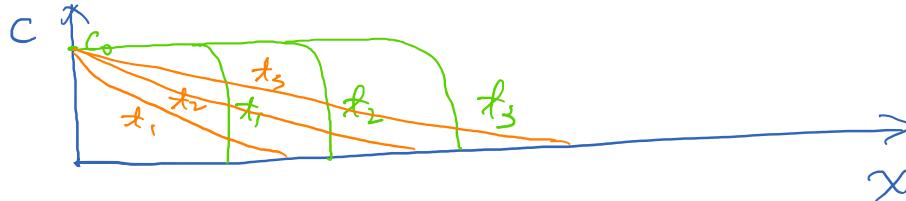
$$Pe = \frac{\text{Advection transport rate}}{\text{Dispersive transport rate}} = \frac{\text{Dispersive time scale}}{\text{Advection time scale.}}$$

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

- 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)

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

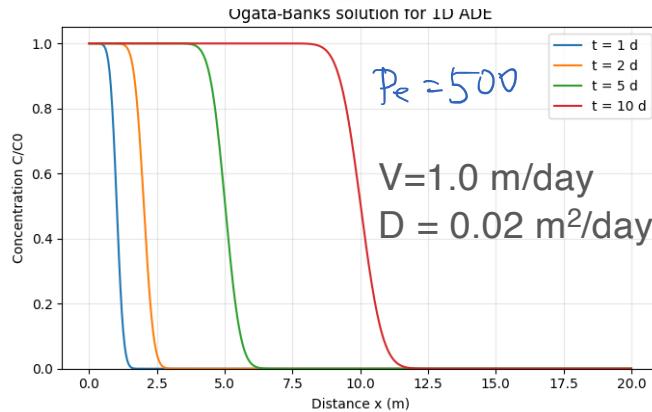
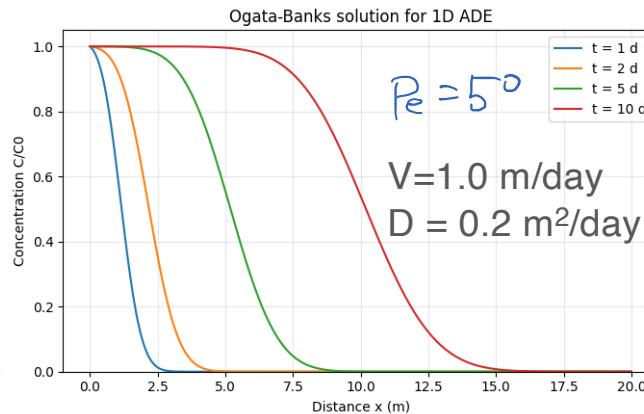
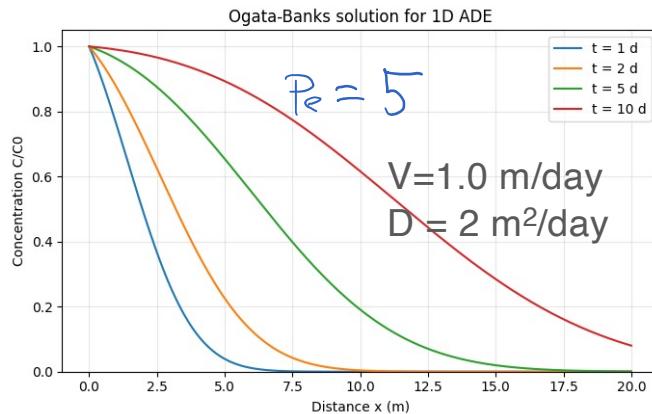
$$C(\infty, t) = 0, t \rightarrow \infty$$

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

[Ogata and Banks, 1961]

# 1D step change in concentration

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



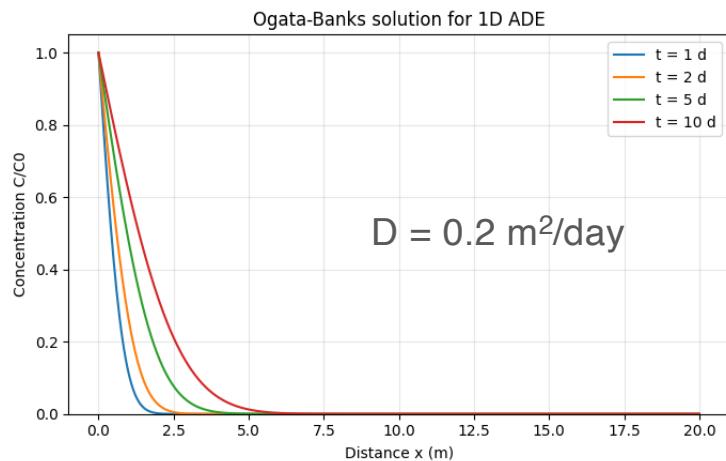
$$\text{Pe} = \frac{VL}{D}$$

$L = 10$

# 1D step change in concentration

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

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



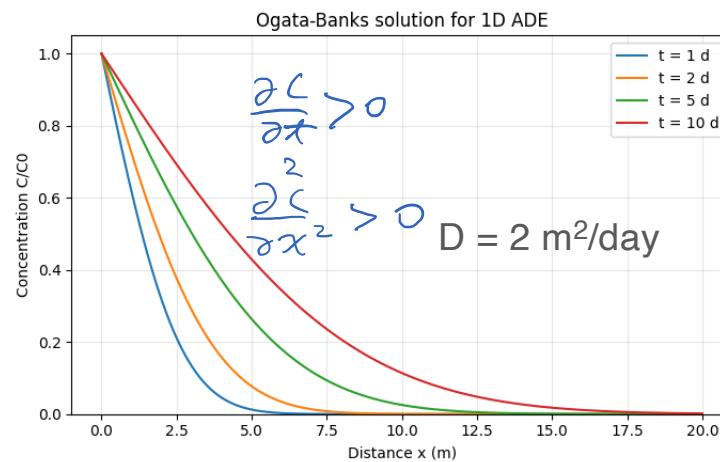
$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2}$$

Gaussian distribution

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

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

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



# 1D step change in concentration

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Characteristic time scales for advection and dispersion

# 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

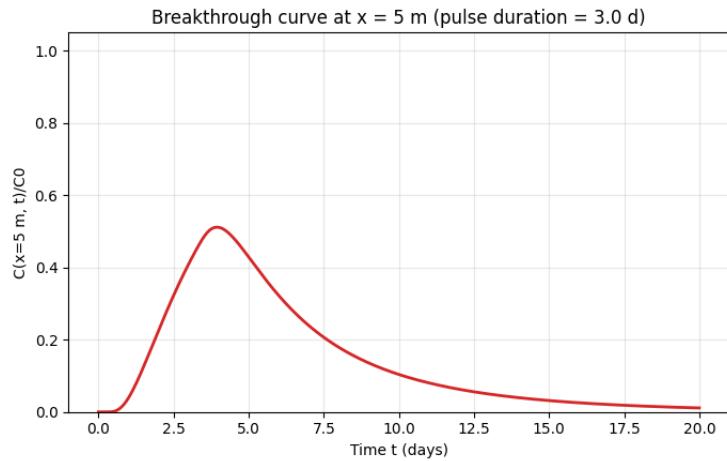
$$0 \leq t < t_0$$

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

$$t \geq t_0$$

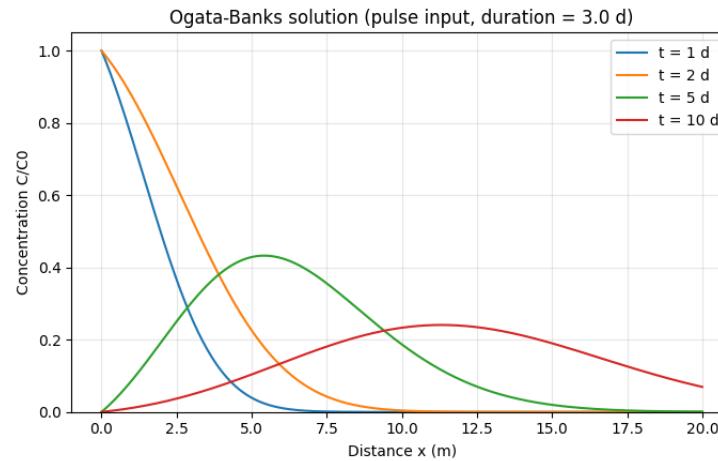
$$C = F(x, t) - F(x, t - t_0)$$

# Moment analysis



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

Total mass passing the observation point.



Pulse injection

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

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

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

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

Total mass in the system at a given time.

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

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

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

# 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.
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
		Plume asymmetry in space
		$M_s^3 = \frac{\int_0^\infty (x - M_s^1)^3 C dx}{M_s^0}$
		Plume intermittency and extreme spreading
		$M_s^4 = \frac{\int_0^\infty (x - M_s^1)^4 C dx}{M_s^0}$

# 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.

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

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

# 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)

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

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

[van Genuchten, 1981]