

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)

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

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

$$\frac{\partial c}{\partial t} = \frac{\partial(\tilde{c}c_0)}{\partial(\tilde{t}L/v)} = \frac{vc_0}{L} \frac{\partial \tilde{c}}{\partial \tilde{t}}$$

$$v \frac{\partial c}{\partial x} = v \frac{\partial(\tilde{c}c_0)}{\partial(\tilde{x}L)} = \frac{vc_0}{L} \frac{\partial \tilde{c}}{\partial \tilde{x}}$$

$$D \frac{\partial^2 c}{\partial x^2} = D \frac{\partial^2(\tilde{c}c_0)}{\partial(\tilde{x}L)^2} = \frac{Dc_0}{L^2} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}^2}$$

$$\frac{vc_0}{L} \frac{\partial \tilde{c}}{\partial \tilde{t}} + \frac{vc_0}{L} \frac{\partial \tilde{c}}{\partial \tilde{x}} - \frac{Dc_0}{L^2} \frac{\partial^2 \tilde{c}}{\partial \tilde{x}^2} = 0$$

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

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:

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

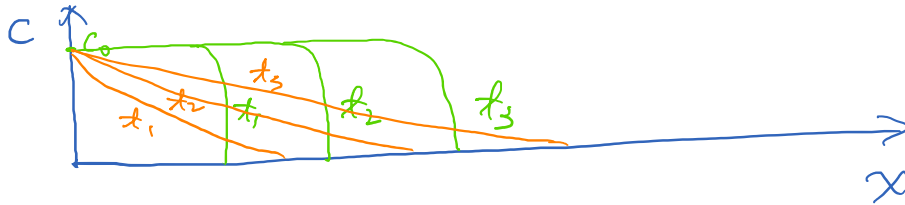
$$\left. \begin{aligned} t_{\text{Adv}} &= L/v \\ t_{\text{Disp}} &= L^2/D \end{aligned} \right\} \Rightarrow Pe = \frac{L^2/D}{L/v} = \frac{vL}{D}$$

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

1D step change in concentration

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Let us first consider a semi-infinite domain.



Initial condition

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

Boundary conditions (assuming semi-infinite domain)

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

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

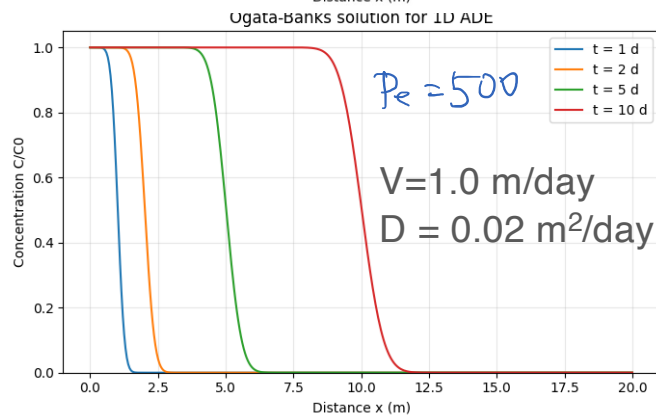
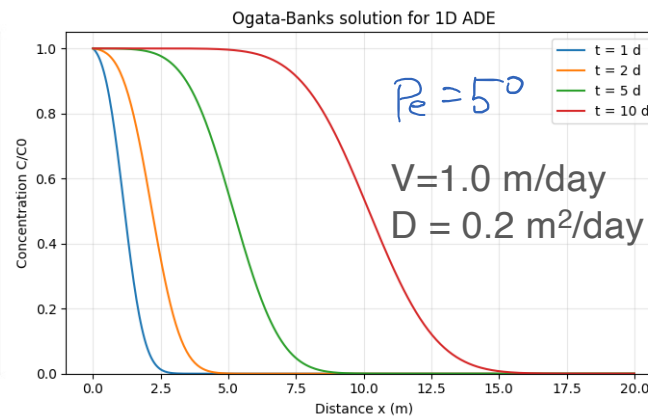
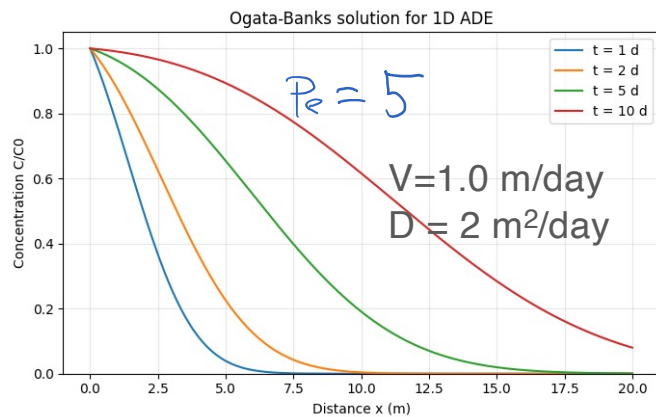
$$C = \frac{C_0}{2} \left[\operatorname{erfc} \left(\frac{x - Vt}{2\sqrt{Dt}} \right) + \exp \left(\frac{VL}{D} \right) \operatorname{erfc} \left(\frac{x + Vt}{2\sqrt{Dt}} \right) \right]$$

[Ogata and Banks, 1961]

1D step change in concentration

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



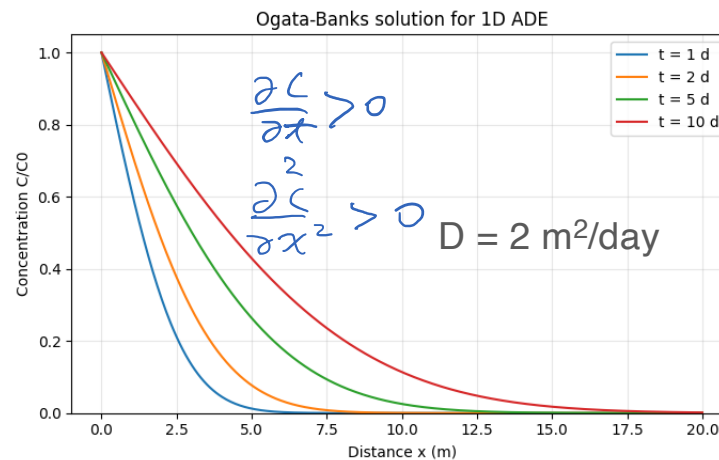
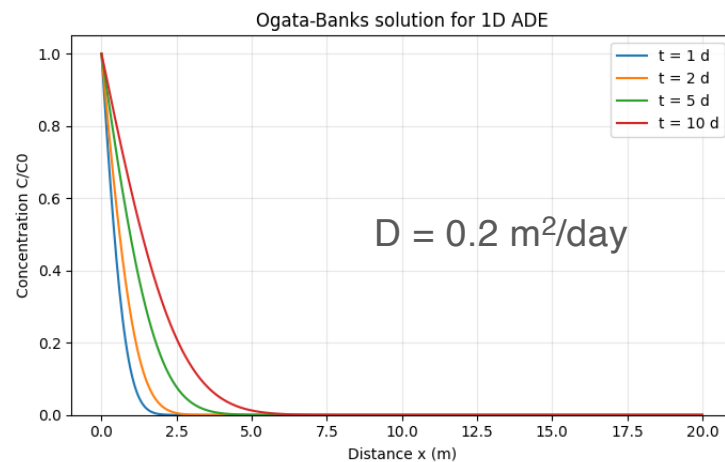
$$Pe = \frac{VL}{D}$$

$L = 10$

1D step change in concentration

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

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



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



1D step change in concentration

Characteristic time scales for advection and dispersion

1D pulse change in concentration

Pulse change in concentration

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

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

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

$$0 \leq t < t_0$$

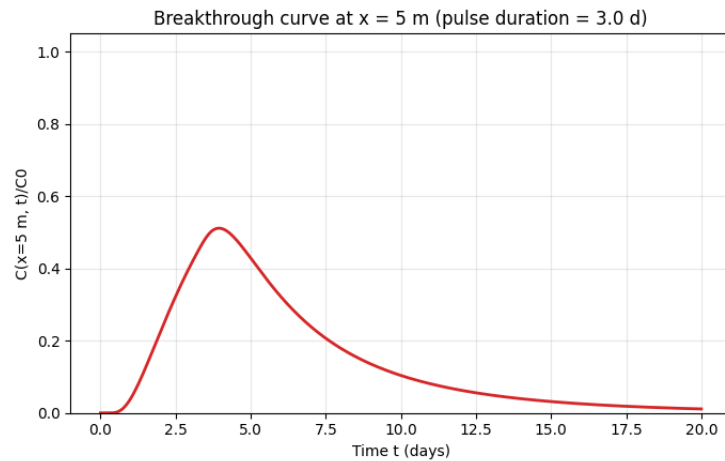
$$C = F(x, t)$$

$$t \geq t_0$$

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

Moment analysis

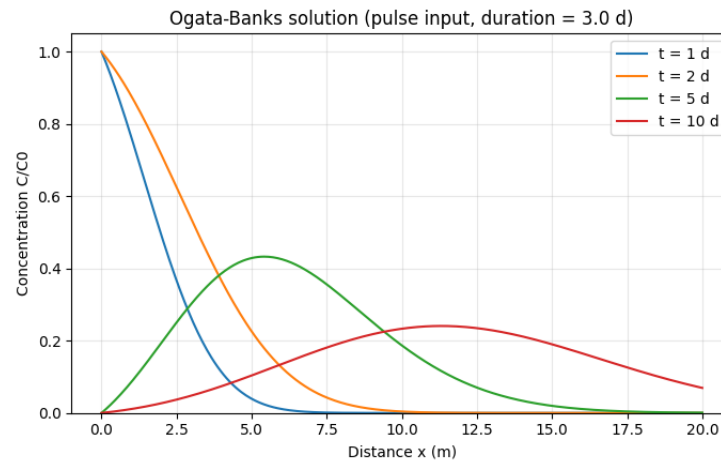
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$$M_t^0 = \int_0^\infty C dt \quad \text{Total mass passing the observation point.}$$

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

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



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

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

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

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

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

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

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)

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

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

[van Genuchten, 1981]