Lecture Modellierung von Hydrosystemen

Mass Transport Process Part I

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Outline

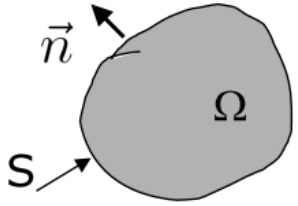
- Advection – Diff. / Disp. – Equation (ADE)
- Dispersion and Diffusion
- Sorption Isotherms and Decay
- Exercise on the mass transport simulation

Governing Equations

If you can only remember one equation, then the Reynolds Transport Theorem.

$$\frac{\partial}{\partial t}\int_{\Omega}\psi\, d\Omega = -\oint_{\partial\Omega}\mathbf{\Phi}^{\psi}\cdot d\mathbf{S} + \int_{\Omega} q^{\psi}\, d\Omega \qquad \text{(Eq. 0)}$$

Or, you can remember a story.



{ Rate of accumulation for unknown Ψ within the volume Ω } = { Net influx of Ψ into the volume Ω through its surface S } + { Net rate of Ψ production within the volume Ω }

Governing Equations

Because of the Gauss Divergence Theorem.

$$\oint_{\partial\Omega} \Phi^{\psi} \cdot dS = \oint_{\Omega} \nabla \cdot \Phi^{\psi} d\Omega$$

So, our Eq. 0 becomes.

$$\frac{\partial}{\partial t} \int_{\Omega} \psi d\Omega = - \int_{\Omega} \nabla \cdot \Phi^{\psi} d\Omega + \int_{\Omega} q^{\psi} d\Omega \qquad \text{(Eq. 1)}$$

Advection Dispersion Equation (ADE)

If write Eq. 1 in derivative form,

$$\frac{\partial \psi}{\partial t} = \nabla(\Phi) + Q \qquad \text{(Eq. 2)}$$

Our primary unknown is Mass

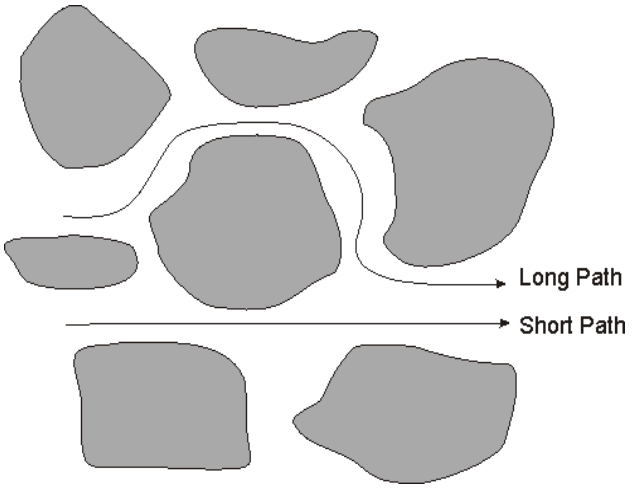
$$\psi = n_e C dA$$

Our flux is composed of:

1) Advective flux

2) Diff./ Disp. flux

Source / Sink



Advection (Mass takes a free ride)

Flux of advection $F_{adv} = v_i n_e C dA$

Average Linear Velocity $v_x = -\frac{K}{n_e}\frac{dh}{dl}$

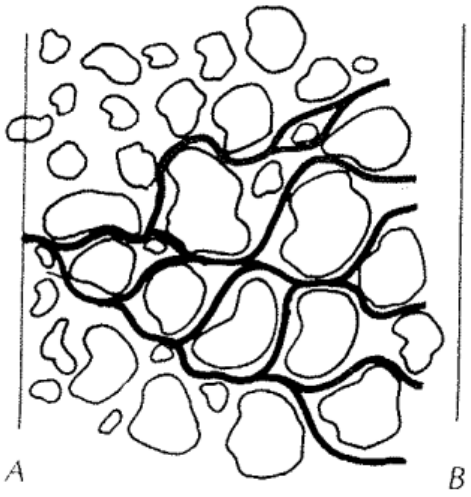
AKA, Pore Velocity $v_x = \frac{q}{n_e}$

q ← Flux

n_e ← Effective porosity

Velocity of a conservative tracer.

Advection Dispersion Equation (ADE)



Dispersion

Diff./ Disp. Flux (Fick's 1st Law)

$$F_{dis/diff} = -D\frac{dC}{dx}$$ 1D

$$F_{dis/diff} = -D \bigtriangledown (C)$$ 3D

Think about:

Why negative sign?

Hydrodynamic Dispersion (Mechanical spreading)

$$D_L = \alpha_L v_i + D^*$$

$$D_T = \alpha_T v_i + D^*$$

Diffusion coefficient

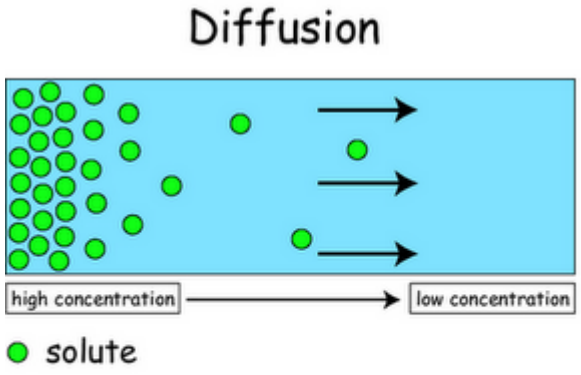
Longitudinal / transverse dispersivity

Note: Dispersivity values are often scale dependent!

$$\alpha_L = 0.83(logL)^{2.414}$$ Xu and Eckstein (1995)

Xu and Eckstein (1995) Use of weighted least-squares method in evaluation of the relationship between dispersivity and field scale. Ground Water 33, no. 6: 905-08

Advection Dispersion Equation (ADE)



Solute transport is from the left to the right; movement of the solutes is due to the concentration gradient (dC/dx).

Diffusion (Molecular spreading)

- It is orders magnitudes lower than dispersion effect.
- Does not dependent on the flow process.
- It is largely temperature dependent.

Putting advection and dispersion into Eq. (2).

We get the governing equation for the mass transport process:

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} - D\frac{\partial^2 C}{\partial x^2} = Q$$

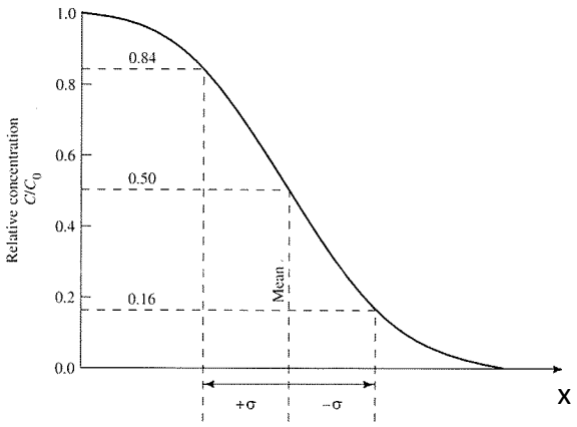
Diffusion of ions in sea water and in deep-sea sediments 705

Table 1. Tracer and self-diffusion coefficients of ions at infinite dilution

Cation	D_j^0 (10^{-6} cm²/sec) 0°C	18°C	25°C	Anion	D_j^0 (10^{-6} cm²/sec) 0°C	18°C	25°C
H^+	56·1	81·7	93·1	OH^-	25·6	44·9	52·7
Li^+	4·72	8·69	10·3	F^-	—	12·1	14·6
Na^+	6·27	11·3	13·3	Cl^-	10·1	17·1	20·3
K^+	9·86	16·7	19·6	Br^-	10·5	17·6	20·1
Rb^+	10·6	17·6	20·6	I^-	10·3	17·2	20·0
Cs^+	10·6	17·7	20·7	IO_3^-	5·05	8·79	10·6
NH_4^+	9·80	16·8	19·8	HS^-	9·75	14·8	17·3
Ag^+	8·50	14·0	16·6	S^{2-}	—	6·95	—
Tl^+	10·6	17·0	20·1	HSO_4^-	—	—	13·3
$Cu(OH)^+$	—	—	8·30	SO_4^{2-}	5·00	8·90	10·7
$Zn(OH)^+$	—	—	8·54	SeO_4^{2-}	4·14	8·45	9·46
Be^{2+}	—	3·64	5·85	NO_2^-	—	15·3	19·1
Mg^{2+}	3·56	5·94	7·05	NO_3^-	9·78	16·1	19·0
Ca^{2+}	3·73	6·73	7·93	HCO_3^-	—	—	11·8
Sr^{2+}	3·72	6·70	7·94	CO_3^{2-}	4·39	7·80	9·55
Ba^{2+}	4·04	7·13	8·48	$H_2PO_4^-$	—	7·15	8·46
Ra^{2+}	4·02	7·45	8·89	HPO_4^{2-}	—	—	7·34

Li Yuan-Hui, Sandra Gregory (1974) Diffusion of ions in sea water and in deep-sea sediments. *Geochimica et Cosmochimica Acta*, *Volume 38, Issue 5*, *703-714*

Advection Dispersion Equation (ADE) – Analytical Solutions



Complementary Error function

For the governing Equation with only dispersion / diffusion,

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

Analytical solution (Crank 1956)

$$C(x,t) = C_0 \; erfc(\frac{x}{2\sqrt{Dt}})$$

$$erfc(B) = 1 - erf(B)$$

$$erf(B) = \frac{2}{\sqrt{\pi}} \int_0^B e^{-t^2} dt$$

Use a checking table,
Or in Excel and other soft., it is provided.

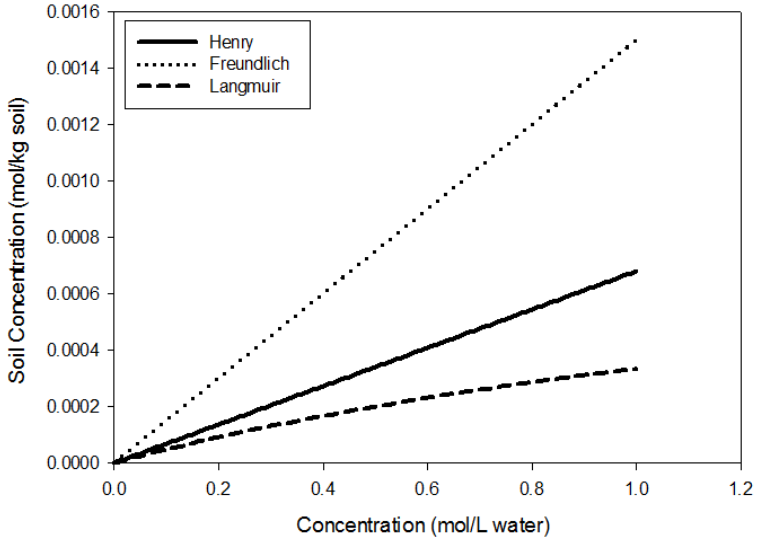
For the Advection - Dispersion / Diffusion equation,

$$\frac{\partial C}{\partial t} + v_x \frac{\partial C}{\partial x} - D\frac{\partial^2 C}{\partial x^2} = Q$$

Analytical solution (Ogata 1970)

$$C(x,t) = \frac{C_0}{2}[\; erfc(\frac{L - v_x t}{2\sqrt{D_L t}}) + exp(\frac{v_x L}{D_L}) erfc(\frac{L + v_x t}{2\sqrt{D_L t}})]$$

Sorption and Decay



Henry $$C^* = K_D C$$

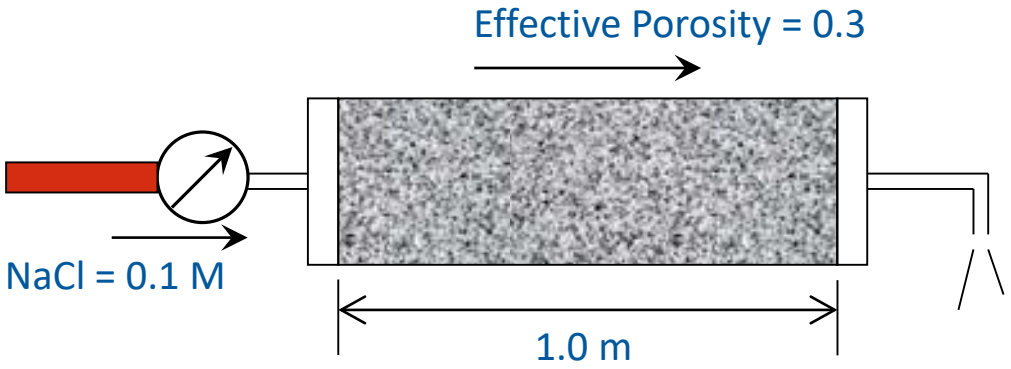
Freundlich $$C^* = K_1 C^{K_2}$$

Langmuir $$C^* = \frac{K_1 C}{1 + K_2 C}$$

1st-order decay $$\frac{\partial C}{\partial t} = -\lambda C$$

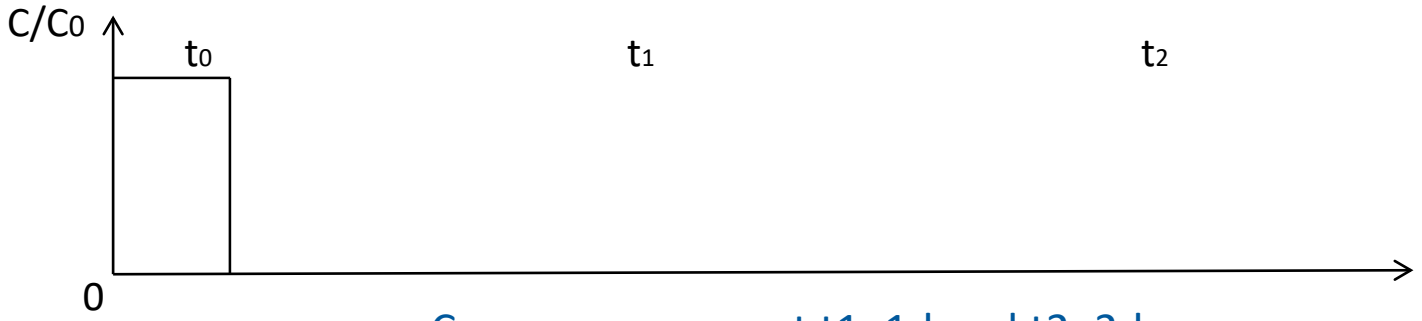
- Soption isotherm describes the distribution of a particular chemical component in the aqueous and solid phase.
- It is called as isotherm because it is measured at a constant temperature.
- Because of different property of the solid phase and sorption component, the isotherm behaves differently and can be described by different mathematical equations.
- Another important behavior of the chemical component is the decay process. Simplest decay process can be described as the first-order decay.
- The radioactive decay exactly follows this decay process.

Exercise



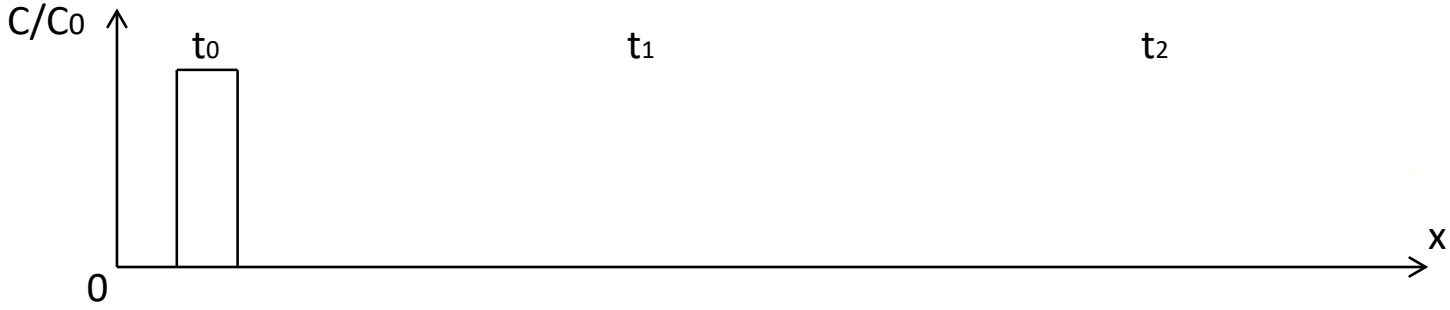
Cross Section Area:
0.001 m2

Q = 0.003 m3/day



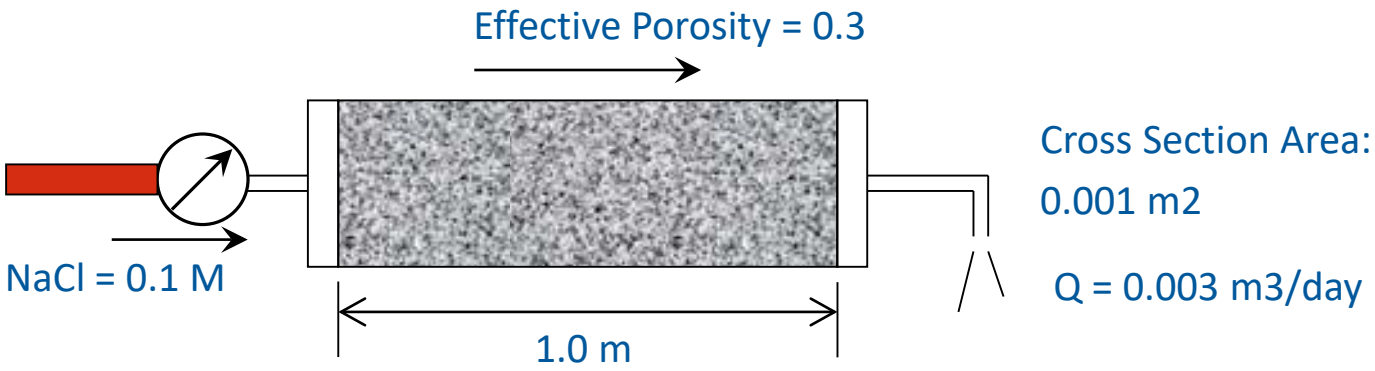
Case (1)
A continuous source

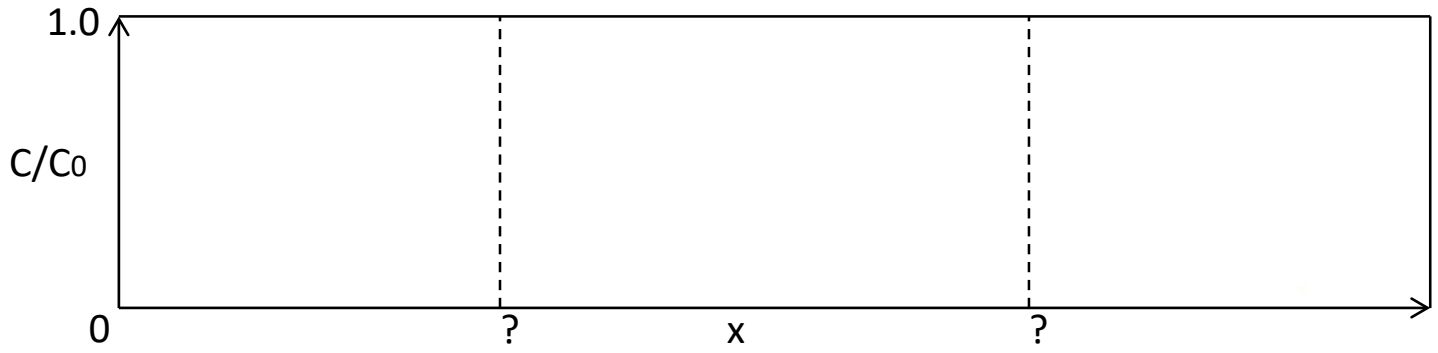
Conc. over space at t1=1d and t2=2d



Case (2)
A shock source

Exercise



Case (3): Assuming soil grain density is 2000 kg/m3, Kd = 2.0 mL/g, how much is the retardation factor R? How does this retardation effect influence the concentration profile?

Case (4): What if there is a 1st order decay on the transported contaminant with (λ = 0.7 1/day)