Reactive Transport in the Hydrosphere

Department of Earth Sciences, Faculty of Geosciences, Utrecht University

Lecturers: Lubos Polerecky and Karline Soetaert

Illustrations, narration and video editing: Renee Hageman
Additional contributions: Dries Bonte, University Ghent
Audio effects: mixkit.co

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Mathematical formulation of transport

Mass balance equation (**1D**-transport):

Rate of change in concentration in **time**

$$\boxed{\frac{\partial C}{\partial t} = R_{Reac} - \frac{1}{A} \cdot \frac{\partial (A \cdot J)}{\partial x}}$$

Net rate of change due to **local reactions**

Rate of change in $A \cdot J$ in **space**

= **Net** rate of change due to **transport**

How do we determine the flux *J*?

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Different modes of transport

I. Advection

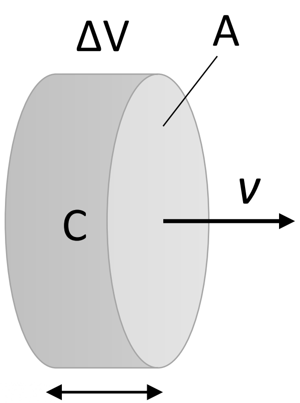
- Occurs due to **directional** movement in space
- Affects solutes and solids
- Examples:
  - Substance dissolved in water + water flow
  - Increase in sediment column height due to sedimentation

mol m^{-2} s^{-1} m s^{-1}

$$\boxed{J_{adv} = v \cdot C}$$

mol m^{-3}

Advective flux:



$\Delta x = v \cdot \Delta t$

- Water volume passing through *A* during Δt:

$$\Delta V = A \cdot \Delta x = A \cdot v \cdot \Delta t$$

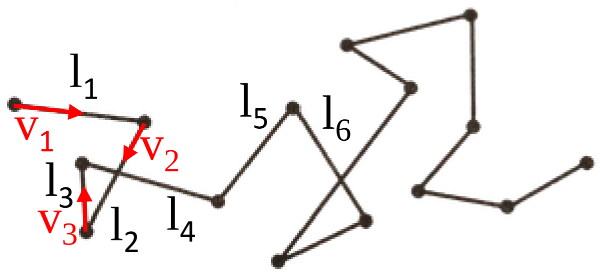
- Amount of substance passing through *A* during Δt:

$$\Delta N = C \cdot \Delta V$$

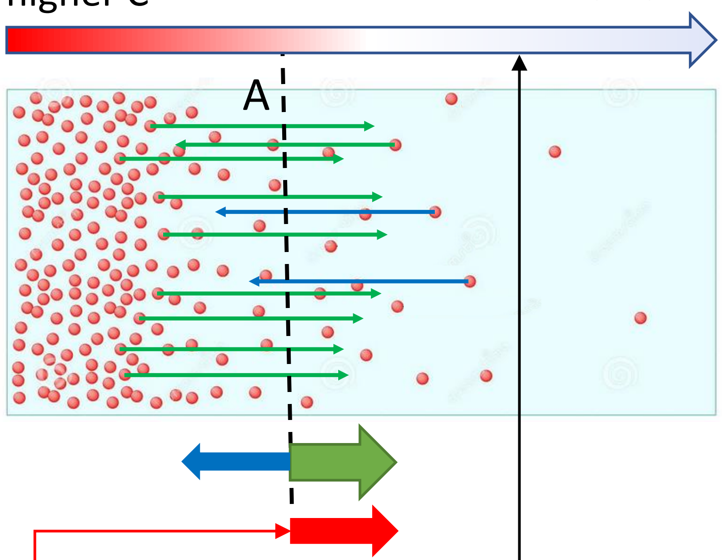
- Flux: $J = \dfrac{\Delta N}{A \cdot \Delta t} = \dfrac{C \cdot \Delta V}{A \cdot \Delta t} = \dfrac{C \cdot A \cdot v \cdot \Delta t}{A \cdot \Delta t} = v \cdot C$

Different modes of transport

II.a **Molecular diffusion**



Brownian motion



Diffusive flux:

Net flux

Fick's law:

$$\boxed{J_{diff} = -D_{mol} \cdot \frac{\partial C}{\partial x}}$$

Concentration **gradient** (mol m^{-4})

Molecular diffusion coefficient (m^2 s^{-1})

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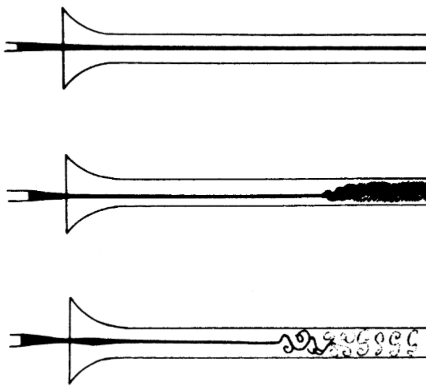
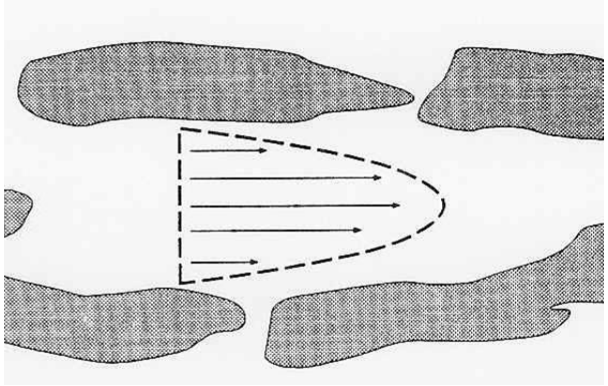
Different modes of transport

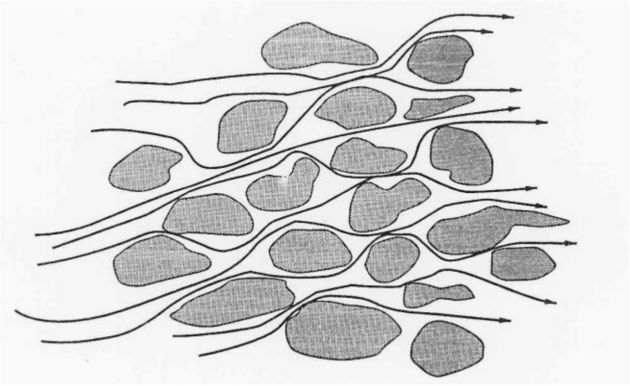
II.b **Dispersion**



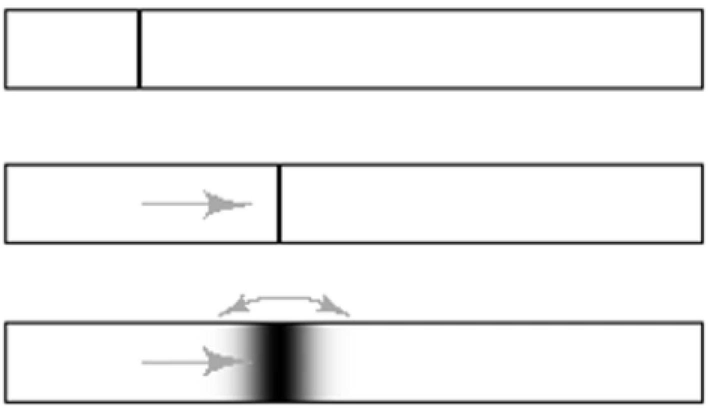
Turbulent flow (Reynolds 1883)



Flow velocity profile



Differences in path-length



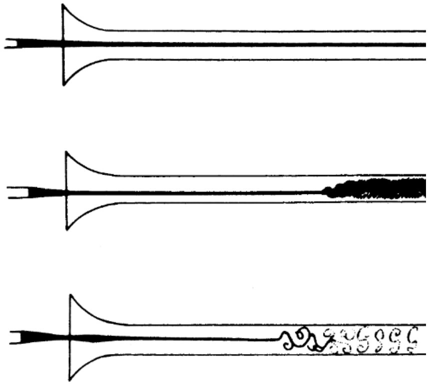
t=0 Dye spill

t>0 Advection but no dispersion

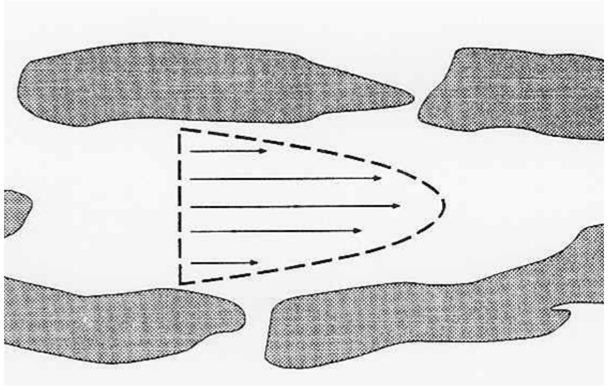
t>0 Advection and dispersion

Different modes of transport

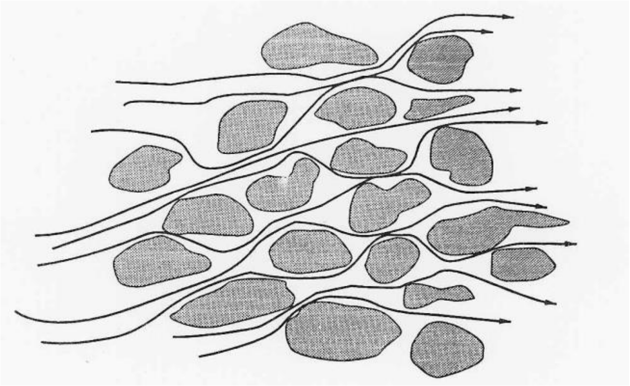
II.b **Dispersion**



Turbulent flow (Reynolds 1883)



Flow velocity profile



Differences in path-length

Dispersive flux

Concentration gradient (mol m^{-4})

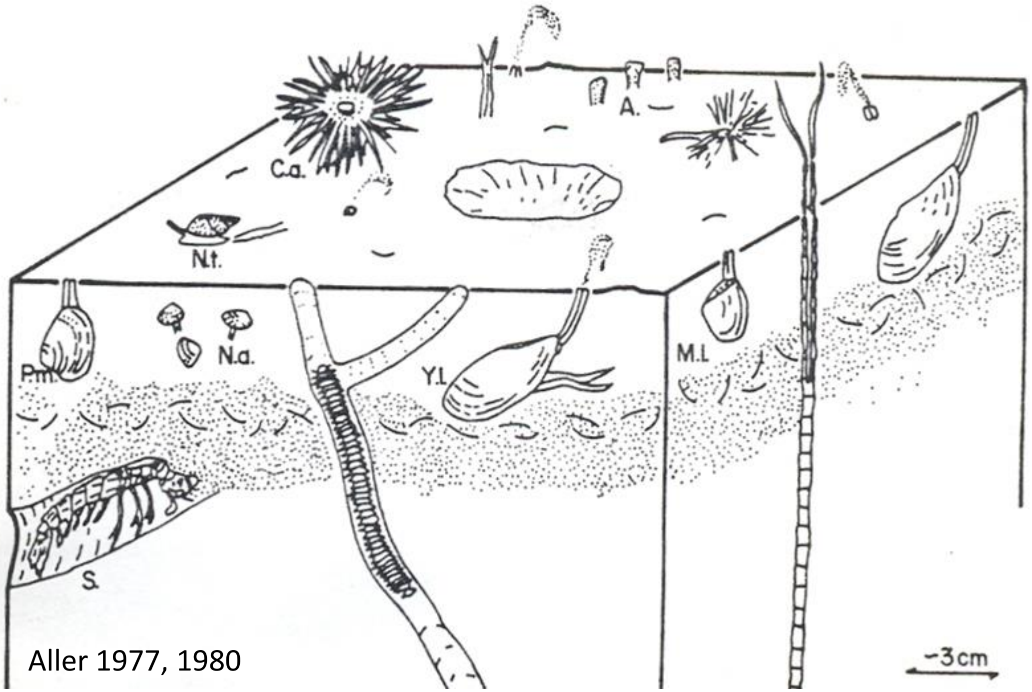
Averaging over scales (temporal & spatial) **much larger** than the scale of **eddies/pores**:

$$J_{disp} = -D_x \cdot \frac{\partial C}{\partial x}$$

Dispersion coefficient (m^2 s^{-1}):

Different modes of transport

II.c **Bioturbation**



Aller 1977, 1980

Short time scales:
Random (Brownian-like) translocation of particles and water packets.

Averaged over sufficiently long time scales:
diffusion-like process!

Bioturbation flux:

$$\boxed{J_{bio} = -D_{bio} \cdot \frac{\partial C}{\partial x}}$$

Bioturbation mixing coefficient ($m^2\ s^{-1}$):

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Different modes of transport

II. Diffusion-like processes

$$J_{diff} = -D \cdot \frac{\partial C}{\partial x}$$

$m^2\ s^{-1} = m \cdot m\ s^{-1}$

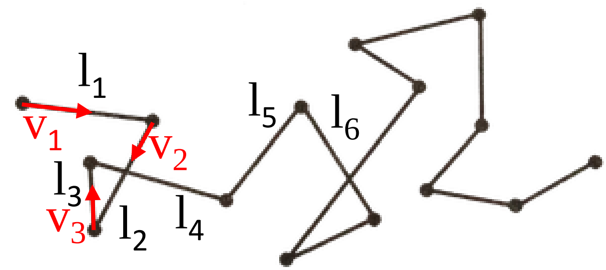
D = characteristic distance (m) · characteristic velocity ($m\ s^{-1}$)

Brownian motion

$$D = \frac{1}{2}\langle l \rangle \cdot \langle v \rangle$$

average **distance** between collisions

average particle **velocity**



Dispersion coefficient

$$D_x = \alpha_L \cdot v_x$$

longitudinal **dispersivity**

bulk water **velocity**

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Dispersion vs. diffusion vs. bioturbation

dispersion

D_{disp}

Horizontal tidal mixing in estuaries:

- $\approx 10 - 100\ m^2\ s^{-1}$

Vertical mixing in oceans, lakes:

- $\approx 0.1 - 1\ m^2\ s^{-1}$

Porewater transport in aquifers:

- $\approx 10^{-6} - 10^{-5}\ m^2\ s^{-1}$

molecular diffusion

D_{mol}

Dissolved gases and other solutes in water:

- $\approx 10^{-9}\ m^2\ s^{-1}$ ($\approx 1\ cm^2\ d^{-1}$)

bioturbation

D_{bio}

Particles in sediments and soils:

- $\approx 10^{-12}\ m^2\ s^{-1}$ ($\approx 1\ cm^2\ yr^{-1}$)

Different modes of transport

Total transport flux (mol m^{-2} s^{-1}):

$$\boxed{J = J_{adv} + J_{diff} = v \cdot C - D \cdot \frac{\partial C}{\partial x}}$$

Due to directional movement

Advection

$$J_{adv} = v \cdot C$$

Bulk velocity (ms^{-1})

Due to random movement

Diffusion-like

$$J_{diff} = -D \cdot \frac{\partial C}{\partial x}$$

$D = D_{disp} + D_{mol} + D_{bio}$ (m^2 s^{-1})

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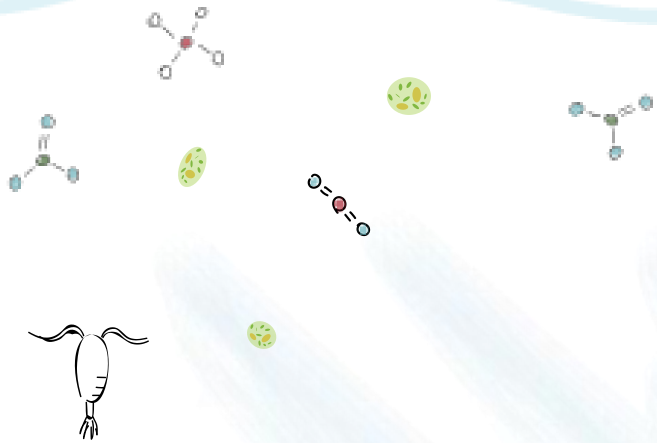

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