Previous Lecture

- **transmissivity**
- **wells – overview**
- **groundwater flow near wells operated at steady state**
- **aquifer characterisation by pumping tests**

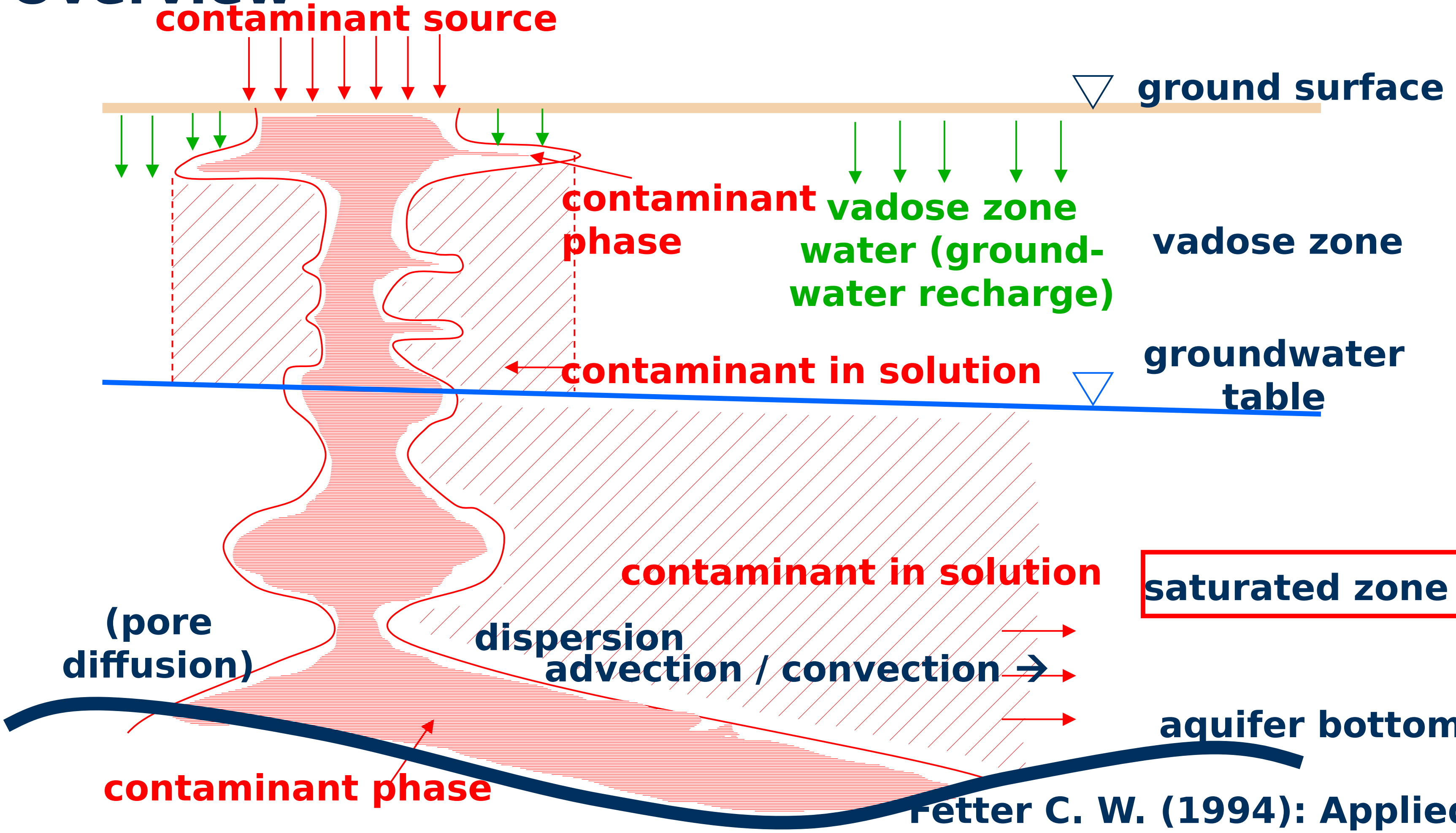
questions?

Today:

- conservative solute transport processes
- joint action of transport processes
- concentration profiles and breakthrough curves

Conservative Solute Transport Processes

Contaminants in Groundwater – Schematic Overview



Fetter C. W. (1994): Applied hydrogeology, Prentice Hall, 3rd ed.

Conservative Solute Transport Processes

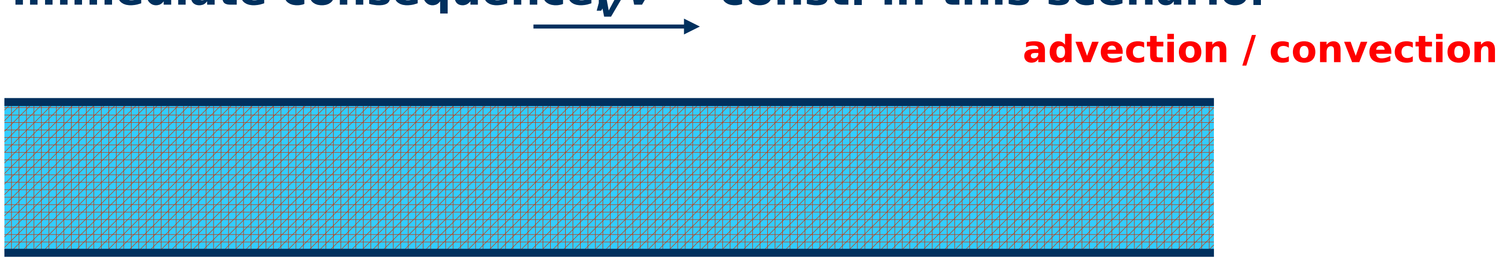
- **This section is intended to cover some basics related to the processes of – advection, – mechanical dispersion, – pore diffusion.**
- **The above processes are summarised as conservative transport processes.**
- **A chemical in groundwater is subject to <u>conservative transport processes</u> if there is – no interaction with the solid material, – no interaction with other chemicals, – no interaction with microbes.**
- **These interactions constitute <u>reactive processes</u>.**
- **For convenience, conservative processes are discussed in the following with regard to 1D scenarios (e.g., Darcy column).**

Advection (Convection)

- <u>Advection</u> (or <u>convection</u>) is the transport of matter or energy *with the movement* of a moving medium.
- The moving medium can be termed carrier. It is usually a fluid.
- Examples:
  - convection of heat (heating circuits, sailplaning)
  - advection of dissolved chemicals or suspended particles in surface or subsurface water or with the wind.
- It seems that the term “convection“ is more frequently used with regard to transport of energy (heat, in particular), while the term “advection“ is more frequently used in connection with the transport of matter.

1D Scenario (Advection)

- 1D flow of a fluid, e.g. water in a lab column filled with a porous medium
- steady-state flow with discharge Q [L³/T]
- cross-sectional area A = const. [L²]
- equation of continuity: $Q = n_e \cdot A \cdot v$ = const.
  with v = linear velocity [L/T] and n_e = effective porosity [-]
- As an immediate consequence, v = const. in this scenario.



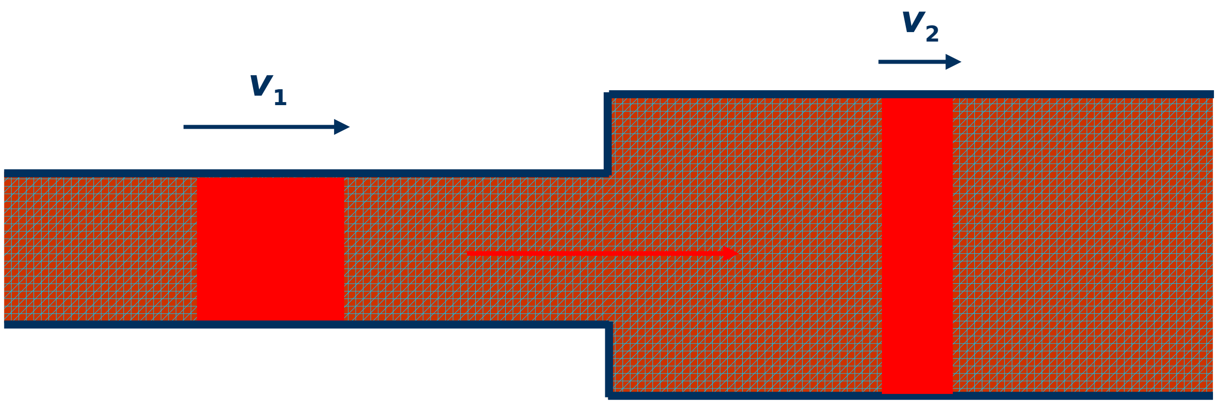
$$J_{adv} = Q \cdot C$$

advective mass flow [M/T]

discharge [L³/T]

solute concentration [M/L³]

Variable Cross Section



$Q_1 = Q_2$

$A_1 \cdot v_1 = A_2 \cdot v_2$

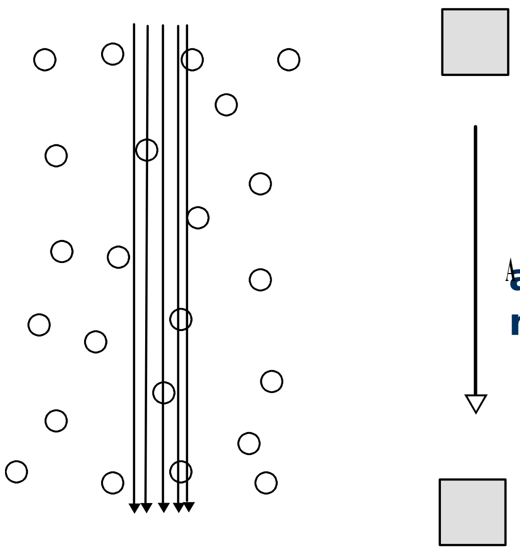
- equation of continuity: $Q = n_e \cdot A \cdot v$ = const.
- According to the equation of continuity, the linear velocity has to be inversely proportional to the cross-sectional area (assuming that effective porosity is spatially constant).
- The mass, which is shown in red, is the same in both flow sections.
- During the transition from the smaller to the larger cross section, the area covered by the solute mass expands laterally and its extension along the flow direction is reduced accordingly.
- The solute concentration is not changed in the red area!

Advection is not Enough …

Plan view!

averaged solute spreading

mittleres Ausbreitungsverhalten

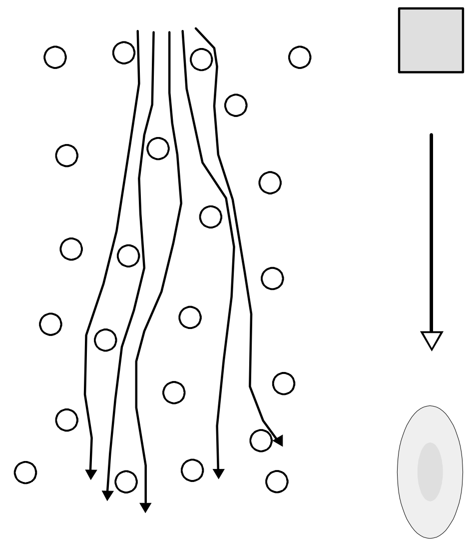


advection

Advektion

actual solute spreading

tatsächliches Ausbreitungsverhalten

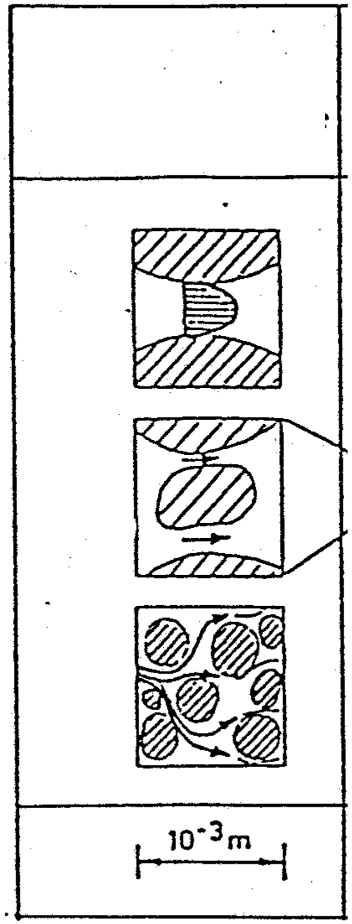


advection + dispersion (longitudinal and transverse)

Advektion + Dispersion ("längs" und "quer")

transverse dispersion is not relevant for 1D problems (e.g., laboratory column)

Mechanical Dispersion



(Kinzelbach, 1992)

Mechanical dispersion is a consequence of

- **different groundwater flow velocities across each individual pore ("parabolic velocity profile"),**
- **different groundwater flow velocities in different pores,**
- **the movement of water around the solids along different flowpaths.**

These effects result in different transport distances and different transport times, respectively, for individual solute particles.

Dispersive Mass Flow due to Mechanical Dispersion

- The dispersive mass flow due to mechanical dispersion in porous media is – proportional to the cross-sectional area, – proportional to the linear velocity, – proportional to the difference in concentration, – inversely proportional to the transport distance.
- The dispersive mass flow is oriented from regions with higher concentrations to regions with lower concentrations.
- Equation:

negative sign!

dispersive mass flow [M/T]

concentration difference [M/L³]

$$J_{disp,m} = - \underline{n_e \cdot A} \cdot \alpha \cdot v \cdot \frac{\Delta C}{L}$$

cross-sectional area [L²]

dispersivity [L]

linear velocity [L/T]

transport distance [L]

Dispersivity and Mechanical Dispersion Coefficient

- **The ratio $\Delta C/L$ is termed <u>concentration gradient</u> [M/L^4].**
- **The dispersivity value equals the value of the dispersive mass flow through a unit cross-sectional area for a unit concentration gradient and a unit linear velocity.**
- **The dimension of dispersivity is length [L]. Dispersivity is a property of the porous medium alone and does not depend on the fluid or the flow behaviour.**
- **The product of dispersivity and linear velocity is called <u>mechanical dispersion coefficient</u>:** $D_{mech} = \alpha \cdot v$
- **The dimension of the mechanical dispersion coefficient is L^2/T. The mechanical dispersion coefficient depends on properties of the porous medium *and* on the flow behaviour.**
- **Dispersive mass flow due to mechanical dispersion can therefore be expressed as:**

$$J_{disp,m} = - n_e \cdot A \cdot D_{mech} \cdot \frac{\Delta C}{L}$$

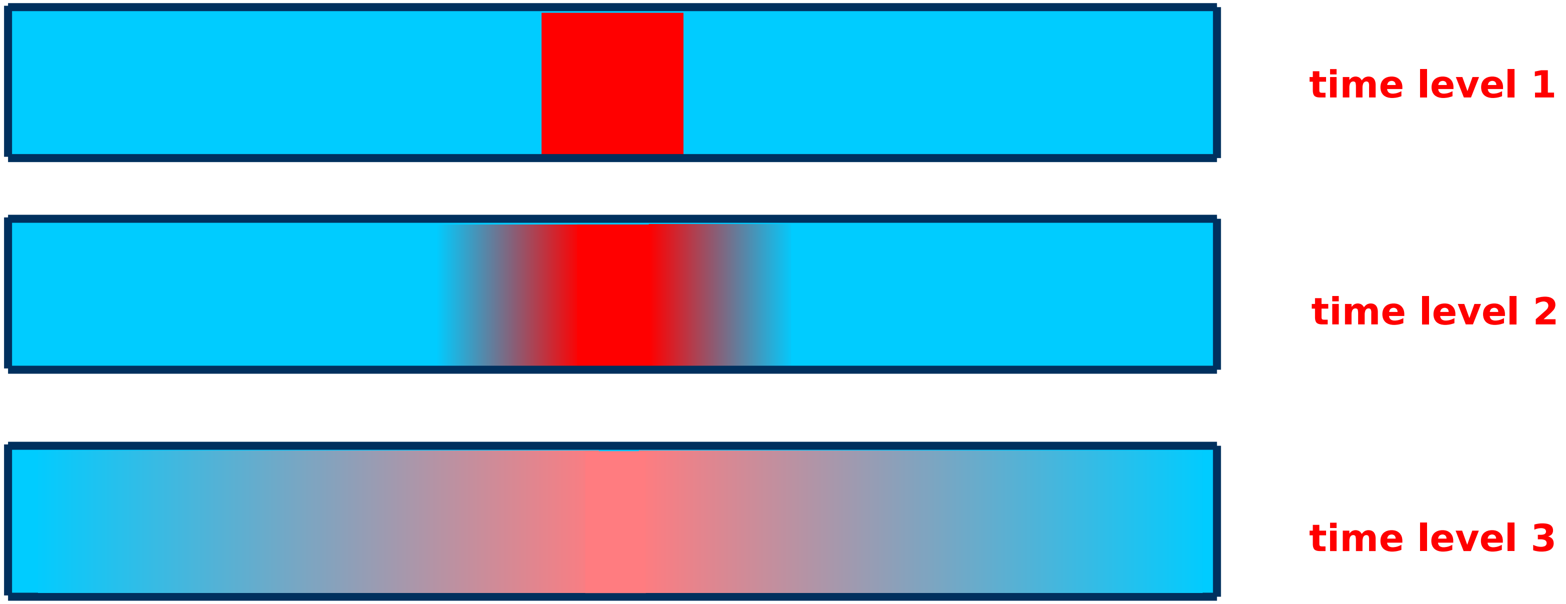
Hydrodynamic Dispersion

- **In addition to mechanical dispersion, concentration gradients are also responsible for solute spreading by diffusion.**
- **The superposition of mechanical dispersion and diffusion is termed <u>hydrodynamic dispersion</u>.**
- **The diffusive mass flow in porous media is not adequately represented by the diffusion coefficient D [L²/T], which is valid for a “free“ fluid.**
- **Rather, the restriction of diffusion by the solids has to be considered.**
- **This is done by introducing the pore diffusion coefficient D_p [L²/T].**
- **General relationship: $D_p < D$**
- **It is frequently assumed that $D_p = n_e \cdot D$ (with n_e = effective porosity) but several other empirical formulae relating D and D_p can be found in literature.**
- **Hydrodynamic dispersion coefficient:**

$$D_{hyd} = D_{mech} + D_p = \alpha \cdot v + D_p = \alpha \cdot v + n_e \cdot D$$

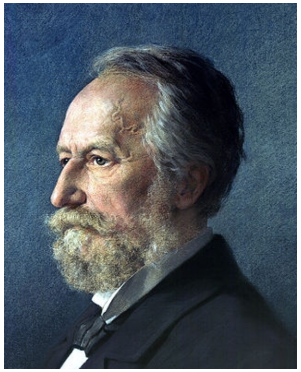
Some Reminders on 1D Diffusion

- 1D diffusion of a dissolved chemical in a fluid, e.g. in water
- no fluid flow, i.e. $Q = 0$ (and consequently $v = 0$)
- Concentration differences are gradually levelled.



Diffusion – Fick‘s First Law

- The mass flow due to 1D diffusion is
  – proportional to the cross-sectional area,
  – proportional to the concentration difference,
  – inversely proportional to the transport distance.
- The mass flow is oriented from regions with higher concen-trations to regions with lower concentrations.
- Fick‘s first law (Fick, 1855):



Adolf Fick
(1829 – 1901)

negative sign!

diffusive mass flow [M/T]

concentration difference [M/L³]

$$J_{diff} = -AD\frac{\Delta C}{L}$$

cross-sectional area [L²]

diffusion coefficient [L²/T]

transport distance [L]

Diffusion Coefficient

- **The dimension of the diffusion coefficient is L^2/T.**
- **The value of the diffusion coefficient equals the value of the diffusive mass flow through a unit cross section for a unit concentration gradient.**
- **Diffusion coefficients for diffusion of dissolved chemicals in water are mostly in the range from 10^{-10} m^2/s to 10^{-9} m^2/s.**
- **Diffusion coefficients for diffusion of dissolved chemicals in gases are larger by about four orders of magnitude, i.e. in the range from 10^{-6} m^2/s to 10^{-5} m^2/s.**

Joint Action of Transport Processes

Advection and Dispersion – Mass Flow

- **Spreading of a conservative solute in an unconsolidated aquifer can be understood as a superposition of advection, mechanical dispersion and pore diffusion.**
- **Equations for the mass flow:**

$$J = J_{adv} + J_{disp,m} + J_{diff} = J_{adv} + J_{disp,h}$$

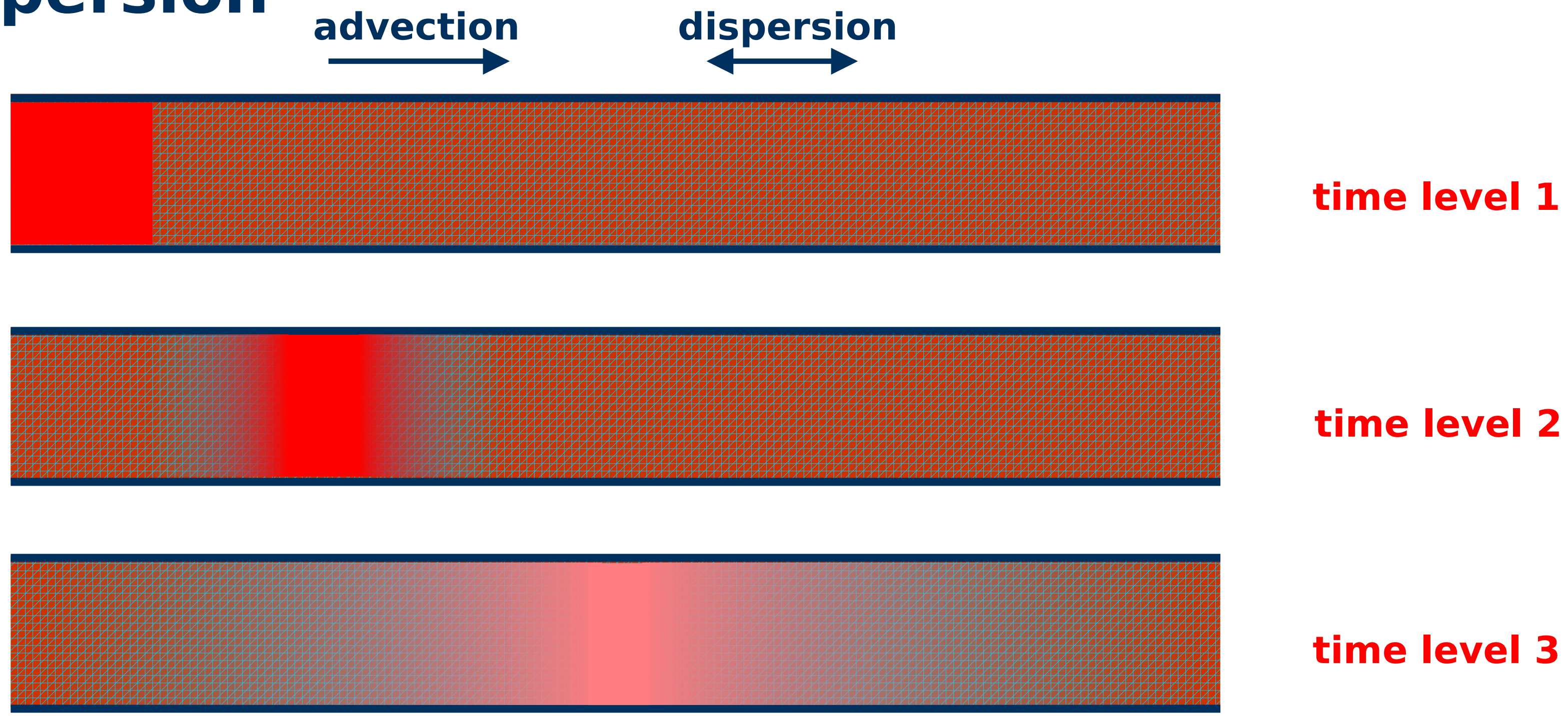
or, alternatively:

$$J = n_e \cdot A \cdot v \cdot C - n_e \cdot A \cdot \alpha \cdot v \cdot \frac{\Delta C}{L} - n_e \cdot A \cdot D_p \cdot \frac{\Delta C}{L} =$$

$$= n_e \cdot A \cdot v \cdot C - n_e \cdot A \cdot D_{hyd} \cdot \frac{\Delta C}{L}$$

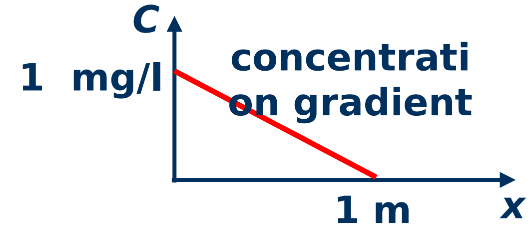
- **The spreading of solutes due to advection and dispersion can be quantified by combining a mass budget and the corresponding laws of motion.**
- **This results in a transport equation (advection-dispersion or convection-dispersion equation) which is discussed a bit in one of the modelling lectures.**
- **The solution of the transport equation is given by the solute concentration *C*(*x*,*t*) which varies in space and time.**

Solute Spreading due to Advection and Dispersion



Relative Importance of Mass Flow Contributions

$$J = n_e \cdot A \cdot v \cdot C - n_e \cdot A \cdot \alpha \cdot v \cdot \frac{\Delta C}{L} - n_e \cdot A \cdot D_p \cdot \frac{\Delta C}{L}$$



cross-sectional area $n_e \cdot A$ **= 1 m²**
linear velocity v **= 1 m/d**
concentration C **= 1 mg/l = 1 g/m³**
transport distance L **= 1 m**
concentration gradient $\Delta C/L$ **= 1 g/m⁴**
dispersivity α **= 0.1 m** **(**$\alpha = L/10$ **is a rough estimate which is frequently used without checking)**
pore diffusion coefficient $D_p = 10^{-10}$ **m²/s**

contribution of advection:

$n_e \cdot A \cdot v \cdot C$ = 1 m² · 1 m/d · 1 g/m³ = 1 g/d

contribution of mechanical dispersion:

$n_e \cdot A \cdot \alpha \cdot v \cdot \Delta C/L$ = 1 m² · 0.1 m · 1 m/d · 1 g/m⁴ = 0.1 g/d

contribution of pore diffusion:

$n_e \cdot A \cdot D_p \cdot \Delta C/L$ = 1 m² · 10^{-10} m²/s · 1 g/m⁴ = 10^{-10} g/s ≈ 10^{-5} g/d

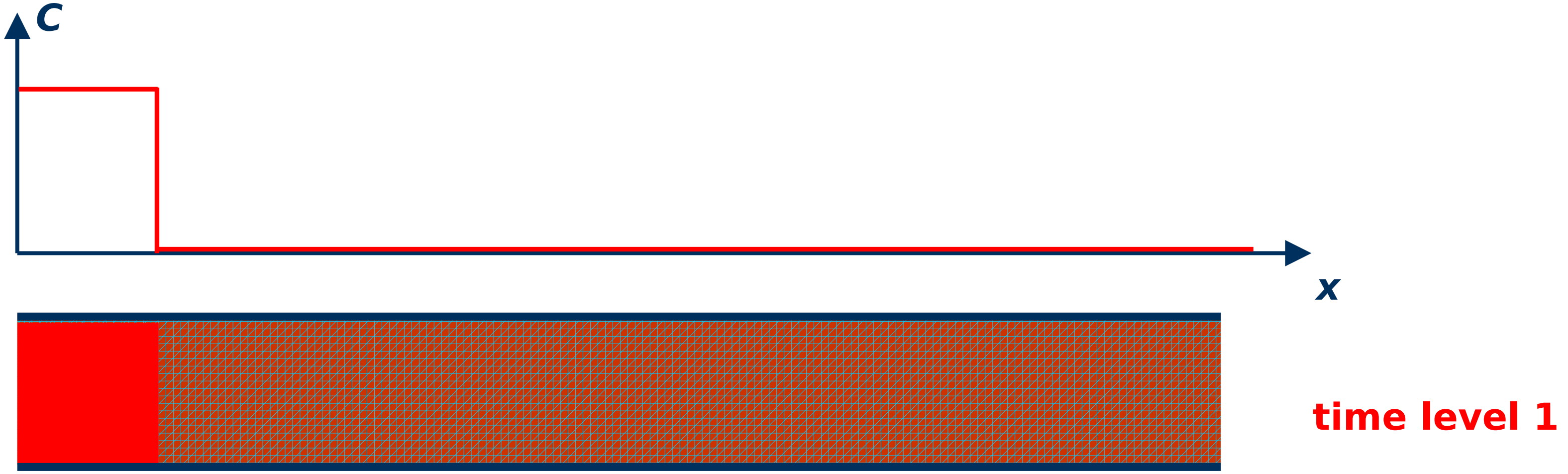
- **advection > mech. dispersion or advection ≈ mech. dispersion**
- **mech. dispersion >> pore diffusion**

(Pore diffusion is usually negligible in unconsolidated aquifers.)

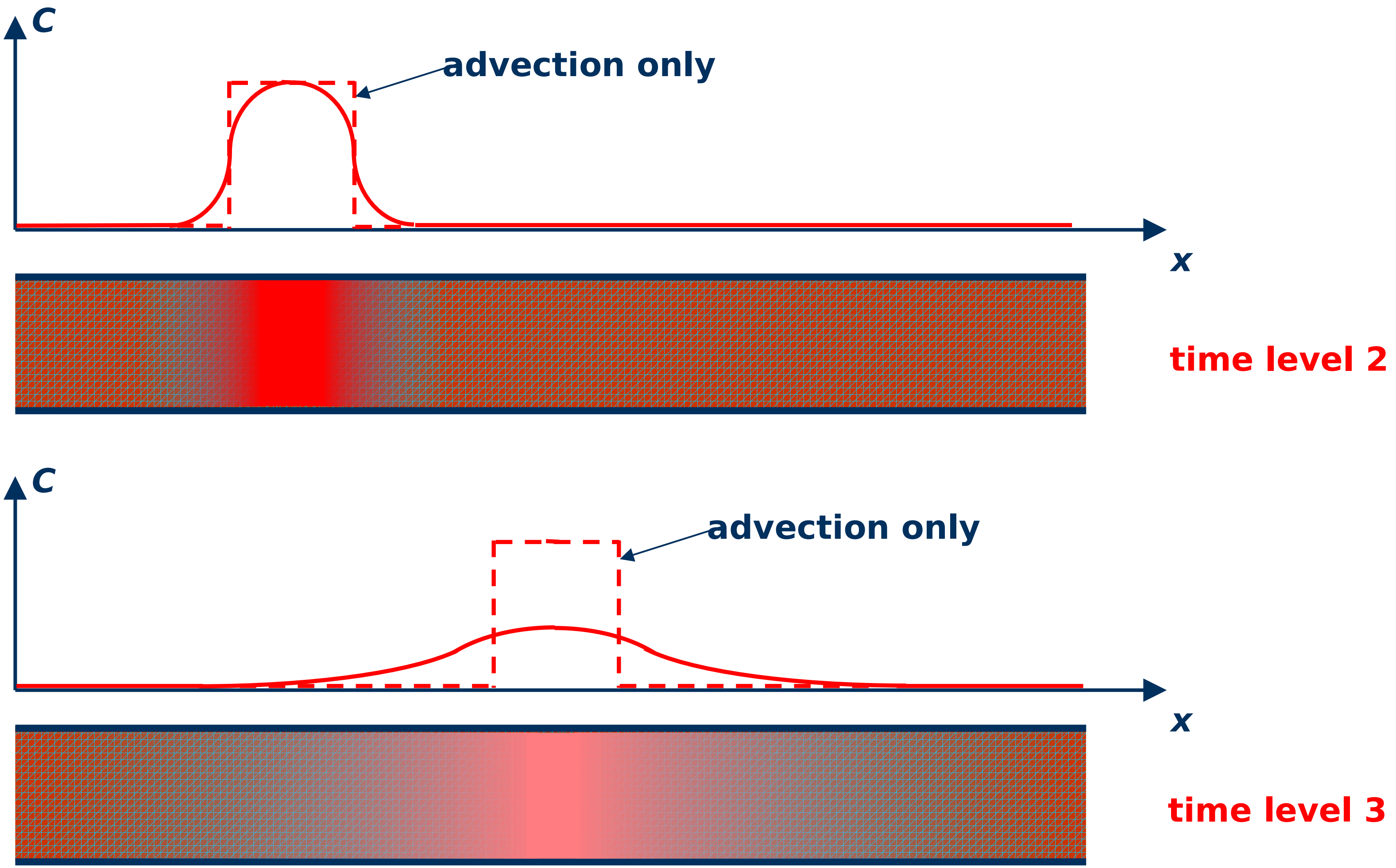
Concentration Profiles and Breakthrough Curves

Concentration Profiles I

<u>Concentration profiles</u> are representations of the solute concentration as a function of a space coordinate at fixed time levels.

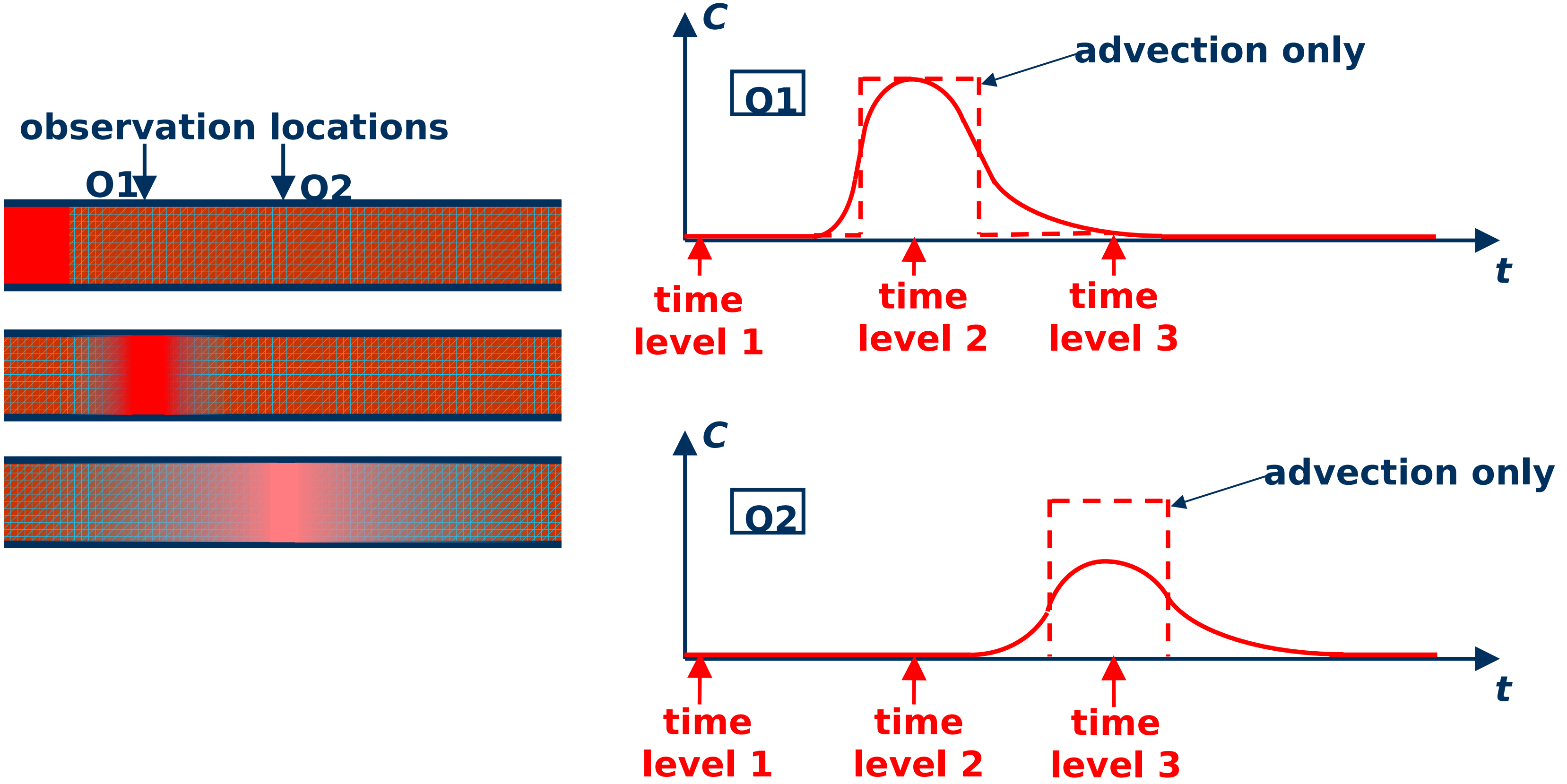


Concentration Profiles II



Breakthrough Curves

<u>Breakthrough curves</u> are representations of the solute concentration as a function of time at specified observation locations.



Excel Worksheet

- 1D solute transport in a porous medium (e.g., laboratory column)
- uniform cross section
- time-invariant water flow
- injection of a tracer
- spreading of the tracer due to advection and mechanical dispersion
- computation and graphical representation of a breakthrough curve based on solutions of the advection-dispersion equation (mass budget & laws of motion)
- comparison with measured data