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Transport processes in rock and soil

Lecture 4

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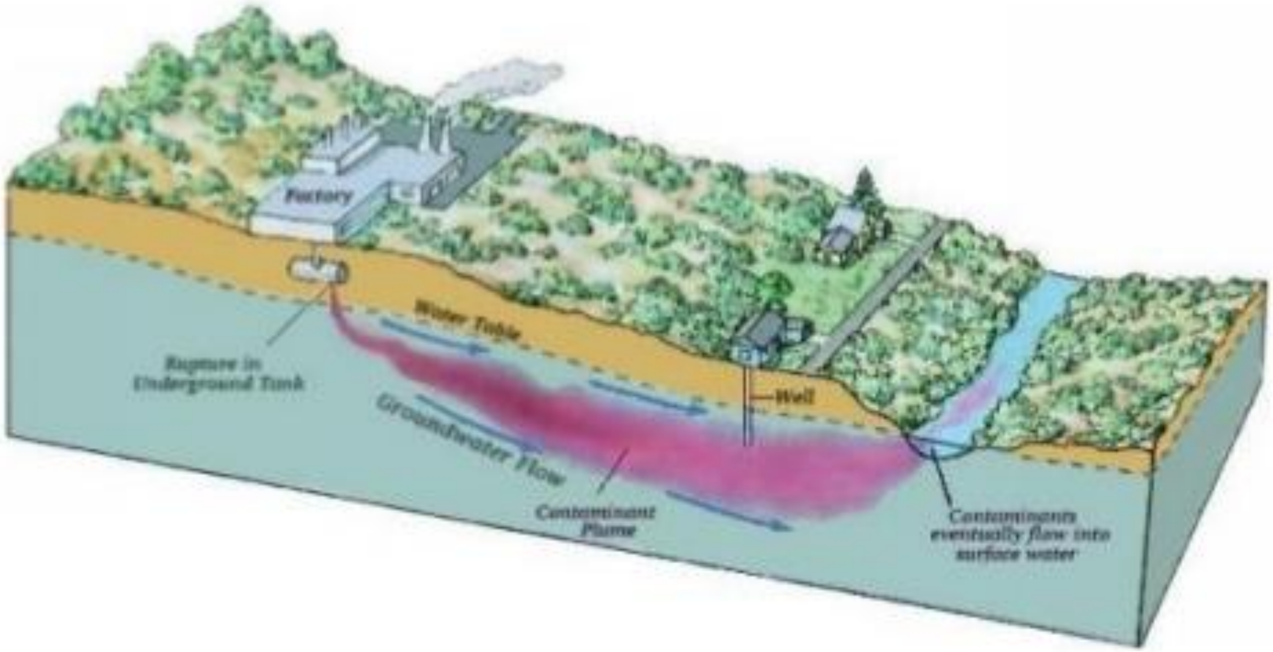
Plan

- Transport of dissolved mass (solute transport)
  - Groundwater contamination, technological processes
  - Fundamentals, equations, parameters
- Different behaviour
  - Scale dependent
    - Transition to REV
  - By parameter relations (process dominance)


Factory
Water Table
Rupture in
Underground Tank
Groundwater Flow
Well
Contaminant
Plume
Contaminants
eventually flow into
surface water

Quantities of solute transport

- System: water + dissolved specie

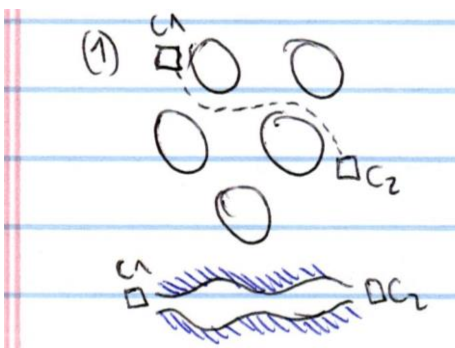
  >>
- C(x,t) concentration = dissolved mass / water volume [kg/m^3]
- Transport mechanisms:
  - With flowing water … advection (convection)
  - Diffusive
- Equation:
  - Fluxes as function of concentration
  - Mass balance
- Mass flux: mass per time per area …. kg/s/m^2
- Advective flux (in sense of REV)

$$\boldsymbol{q}_c^{\mathrm{adv}} = c\boldsymbol{q}$$

Molecular diffusion

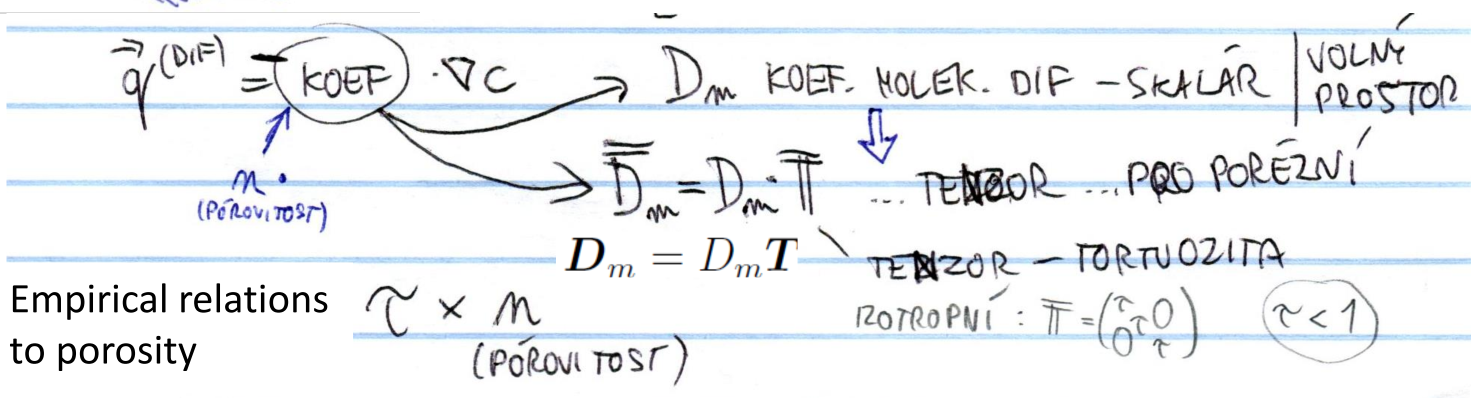
- Free water at rest … Fick's Law … D*grad c …
- Two steps of generalisation
  - Continuous Free space to (homogenized) pores
  - Water at rest to flowing water

$$\frac{\partial c}{\partial t} = D_m \Delta c = D_m \sum_i \frac{\partial^2 c}{\partial x_i^2}$$



Not a direct path …tortuosity

Nonuniform width … constrictivity



$$\boldsymbol{D}_m = D_m \boldsymbol{T}$$

Empirical relations to porosity

Alternative description / parameters of diffusion

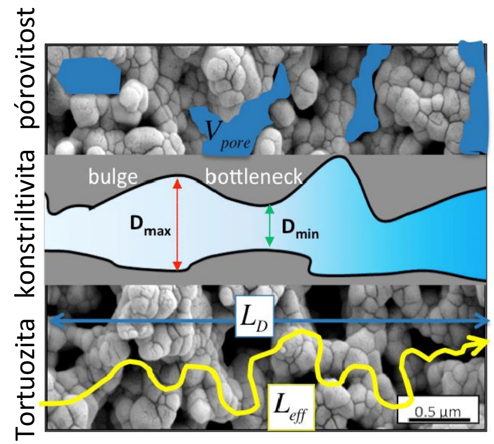
- Simplified
  - Lumped empirical parameter “tortuosity”

$$q_c = -nD_m \tau \nabla c = -n\bar{D}_m \nabla c$$

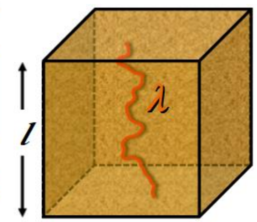
$$\tau < 1 \quad !!!$$

$$\tau \approx \sqrt[3]{n}$$

- Detailed
  - Physical meaning of parameters (but also not measurable)

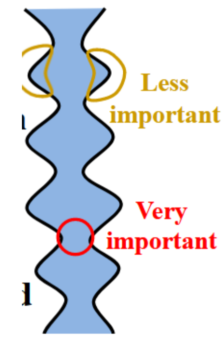


$$\delta(d_{max}, d_{min}) < 1$$



$$\tau = \frac{\lambda}{l} > 1$$

tortuosity



constrictivity

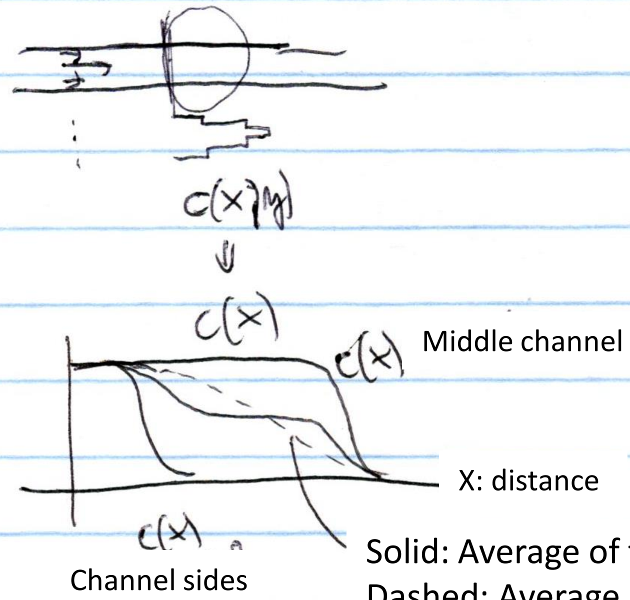
$$q_c = -nD_w \frac{\delta}{\tau^2} \nabla c$$

$$D_p = D_w \frac{\delta}{\tau^2} = GD_w$$

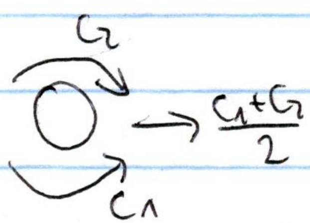
$$D_e = nD_p = nD_w G = F_f D_w$$

D_p pore diffusion c.
D_e effective diff. c.
D_w d.c. in free water
G geometric factor
F_f formation factor

(2) Flowing water in porous medium



Solid: Average of two positions
Dashed: Average across the whole cross-section



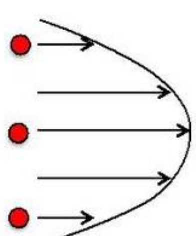
Micro scale:
advection + molecular diffusion

Macro scale:
mixing of individual pores … homogenization

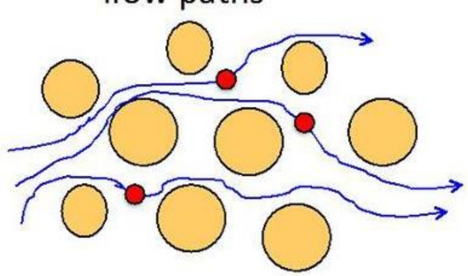
“dispersion”
Mathematically as diffusion … from higher concentration to lower

mechanical dispersion” … just an effect of averaging over REV (homogenization)

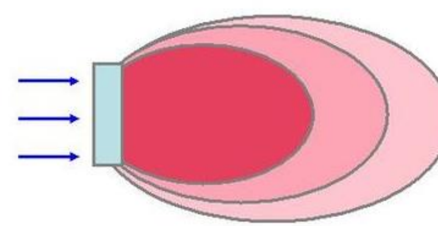
1. Variations in flow velocity



2. Different solute flow paths



3. Causes the plume to spread



Dispersive transport quantification

Same equation, different coefficient … tensor

$$[\boldsymbol{D}_f]_{ij} = \alpha_T.|\boldsymbol{v}|.\delta_{ij} + (\alpha_L - \alpha_T)\frac{v_i\,v_j}{|\boldsymbol{v}|}$$

$[m^2/s]$ $[m]$ $[m/s]$ $[m]$ $[m/s]$

$$\delta_{ij} = \begin{cases} 0 & i \neq j \\ 1 & i = j \end{cases}$$

Kronecker delta (unit matrix written by indices)

$$\vec{v} = (v, 0, 0) \Rightarrow [D_f]_{ij} = 0 \quad i \neq j$$

$$[D_f]_{11} = \alpha_T \cdot v + (\alpha_L - \alpha_T) \cdot v = \alpha_L \cdot v$$

$$_{22} = \alpha_T \cdot v$$

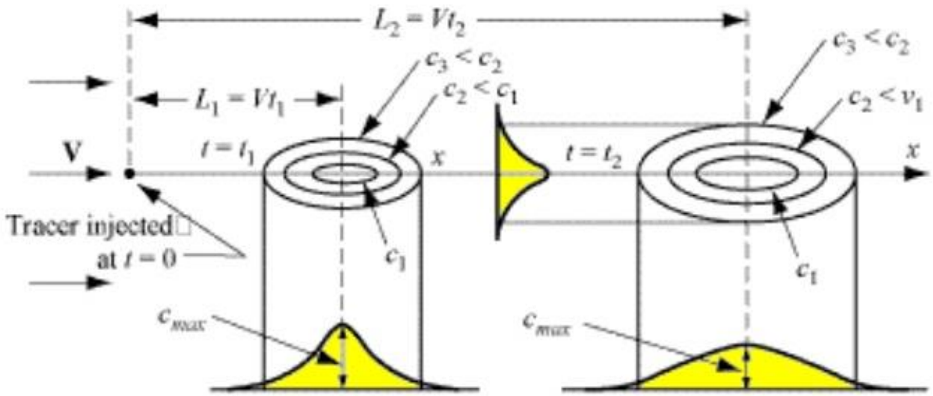
$$_{33} = \alpha_T \cdot v$$

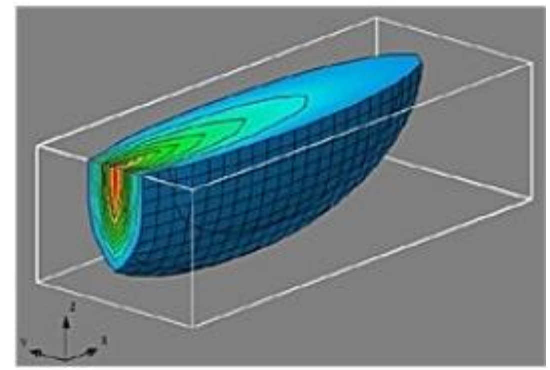
Related to flow velocity direction

$$\begin{bmatrix} \alpha_L \cdot v & 0 & 0 \\ 0 & \alpha_T \cdot v & 0 \\ 0 & 0 & \alpha_T \cdot v \end{bmatrix}$$

Dispersivity:
α_L longitudinal,
α_T transversal

Anizotropic behaviour even for isotropic medium


L2 = Vt2
L1 = Vt1
c3 < c2
c2 < c1
V
t = t1
x
t = t2
x
c3 < c2
c2 < v1
Tracer injected
at t = 0
c1
c1
cmax
cmax



Combination of transport mechanisms – governing equation

- Molecular dif. + mechanical disp.
  = **hydrodynamic dispersion**

$$\boldsymbol{D}_h = \boldsymbol{D}_m + \boldsymbol{D}_f \qquad [\mathrm{m}^2/\mathrm{s}]$$

$$\boldsymbol{q}_c = n(c\boldsymbol{v} - \boldsymbol{D}_h \nabla c)$$

- Balance equation (mass)
  - Change mass = mass flux + sources/sinks

$$\frac{\partial}{\partial t}\int_V nc\,\mathrm{d}V = -\int_{\partial V} \boldsymbol{q}_c \cdot \mathrm{d}\boldsymbol{S} + \int_V (P^+ c^* + P^- c)\,\mathrm{d}V + \int_V r\,\mathrm{d}V$$

With pumping water in/out … given/unknown

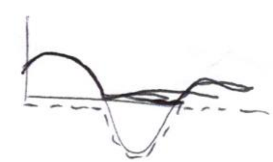
Chemical reaction

$P\left[\frac{m^3}{m^3 s}\right]$

$P = P^+ + P^-$

$P^+ > 0$

$P^- < 0$



Differential equation of solute transport

$$\frac{\partial}{\partial t}\int_V nc\,\mathrm{d}V = -\int_{\partial V}\boldsymbol{q}_c\cdot\mathrm{d}\boldsymbol{S} + \int_V (P^+c^* + P^-c)\,\mathrm{d}V + \int_V r\,\mathrm{d}V$$

$$n\frac{\partial c}{\partial t} + \nabla\cdot(\boldsymbol{q}_c) = P^+c^* + P^-c + r$$

Substitute q_c $$\frac{\partial c}{\partial t} + \nabla\cdot(c\boldsymbol{q}) - n\nabla\cdot(\boldsymbol{D}_h\nabla c) = P^+c^* + P^-c + r$$

Advection-diffusion equation

Divide by n $$\frac{\partial c}{\partial t} = -\nabla\cdot(c\boldsymbol{v}) + \nabla\cdot(\boldsymbol{D}_h\nabla c) + \frac{1}{n}(P^+c^* + P^-c) + \frac{r}{n}$$

Second-order PDE, parabolic type (determined by the diffusion term)

$\boldsymbol{D}_h(\boldsymbol{v})$

Alternative $$n\frac{\partial c}{\partial t} + \nabla\cdot(c\boldsymbol{q}) - \nabla\cdot((\boldsymbol{D}_e + \boldsymbol{D}_f(\boldsymbol{q}))\nabla c) = \ldots(P)\ldots$$

Advection only: $$\frac{\partial c}{\partial t} + \nabla\cdot(c\boldsymbol{v}) = \ldots$$

1st der. 1st der. First-order PDE, hyperbolic type

Analysis of equation properties

Dimensionless number … Péclet

ADVEKČNĚ-DIFUZNÍ ROV. 1D

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} - D_L \frac{\partial^2 c}{\partial x^2} = 0 \quad / :c_0 \quad \cdot L \quad :v$$

$$C = \frac{c}{c_0} \qquad X = \frac{x}{L} \qquad T = \frac{t v}{L}$$

$$\frac{\partial C}{\partial T} + \frac{\partial C}{\partial X} - \frac{D_L}{v \cdot L} \frac{\partial C}{\partial X^2} = 0$$

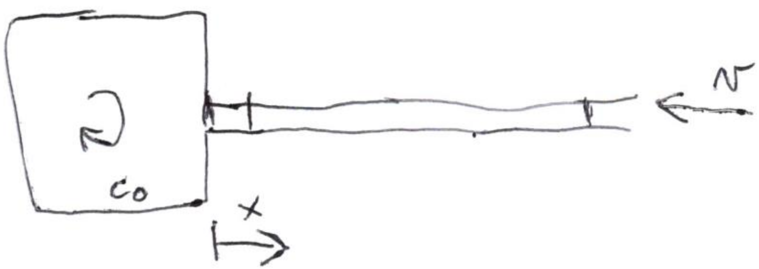
$$\frac{D_L}{v \cdot L} = \frac{1}{Pe} \qquad \frac{m^2/s}{m/s \cdot m} = 1$$

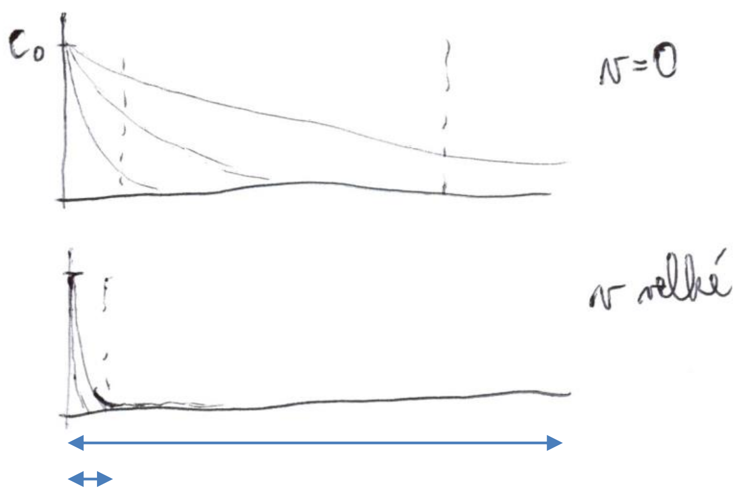
Comparison:
Dominance of either advection of diffusion

Necessary to consider observation scale … characteristic length L

Péclet number demonstration

- Thought experiment: Perfect mixed reservoir and an infinite pipe





Observation scale

Steady state

$$\frac{\partial c}{\partial t} = 0$$

$$0 = -D\frac{\partial c}{\partial x} - vc$$

$$c(x) = c_0 \cdot e^{-\lambda x}$$

Analytical solution of diff. eq.

$$-v\, c(x) - D_h \lambda\, c(x) = 0$$

$$\lambda = -\frac{v}{D_h}$$

$$\frac{c}{c_\infty} = \mathrm{e}^{-\frac{vx}{D}} = \mathrm{e}^{-\mathrm{Pe}}$$

"Pe"

Pe >> 1 ... DOMIN. ADVEKCE

Pe << 1 ... DIFÚZE

Peclet versus Reynolds number

$$\mathrm{Pe} = \frac{v \cdot L}{D_h} \quad \frac{[\mathrm{m/s}][\mathrm{m}]}{[\mathrm{m^2/s}]}$$

$$\mathrm{Re} = \frac{v \cdot L}{\nu} \quad \frac{[\mathrm{m/s}][\mathrm{m}]}{[\mathrm{m^2/s}]}$$

Advection x diffusion

inertial force x internal friction

Analogy?

Viscosity:

force proportional to velocity difference

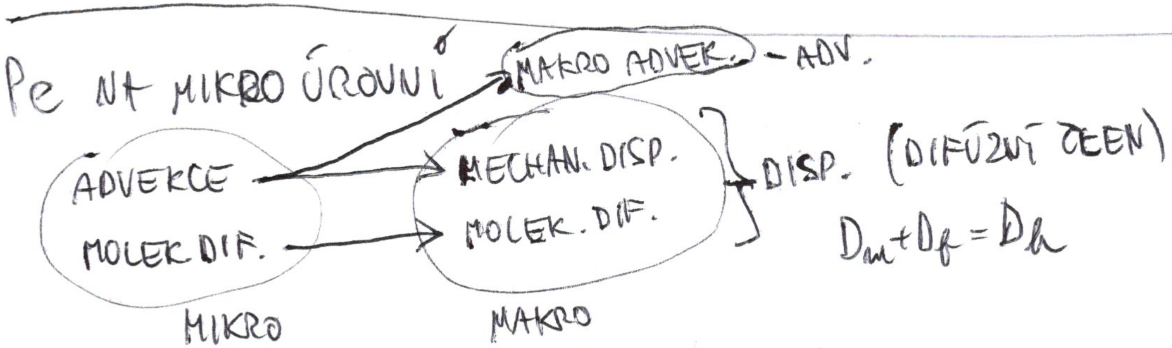
brakes quick particles, accelerates slow particles

“diffusive process”

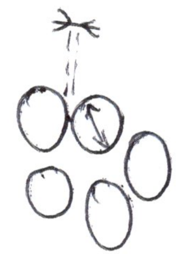
(low Re laminar flow, high Re turbulent flow)

Other Pe context

Pe NA MIKRO ÚROVNI



v versus D_m ← D_m versus D_f



$$Pe = \frac{v \cdot d}{D_m}$$

d… CHARAKT. ROZMĚR ZRN/PÓRŮ

$Pe \ll 1$ DOMIN. D_m

$Pe \gg 1$ D_f

PRO $Pe > 20$ LZE ZANEDBAT D_m