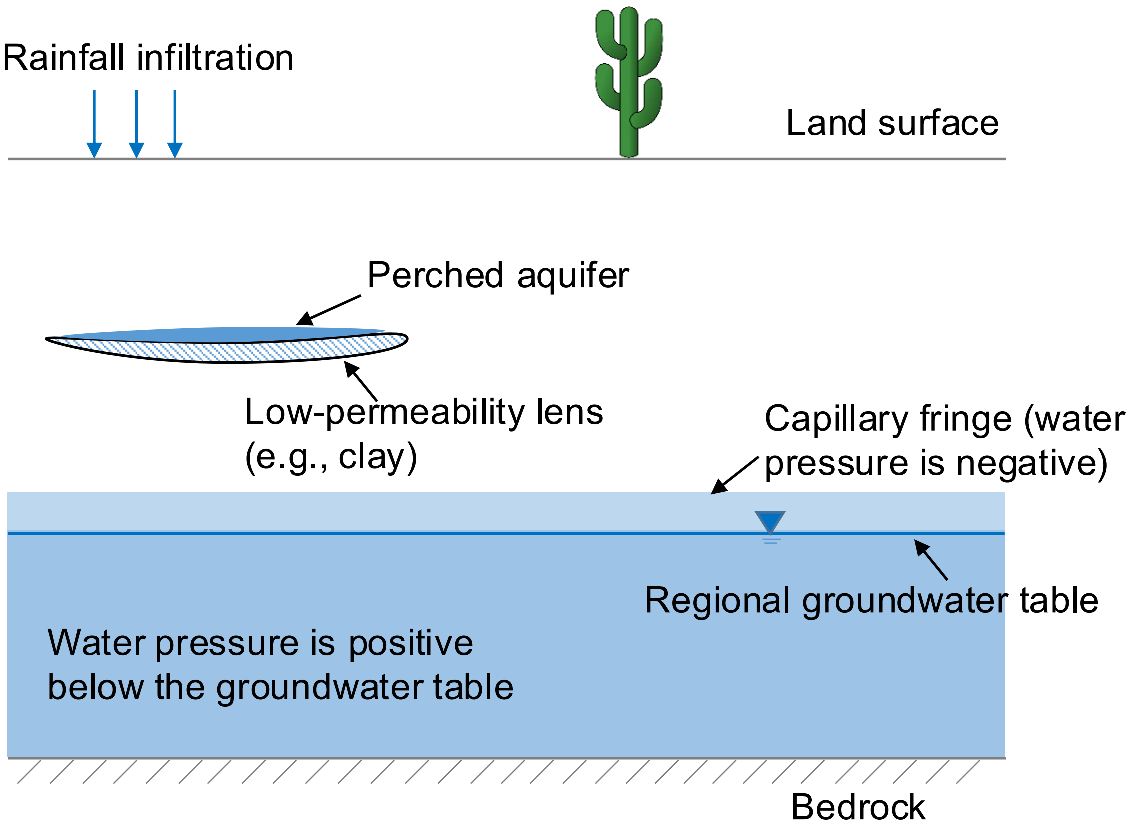
HWRS 561b: Physical Hydrogeology II

Solute transport (Part 1)

Agenda:

1. Overview of the course
2. Review: Steady-state saturated flow
3. Basic concepts for solute transport in saturated porous media

Vadose Zone: Conceptual picture



Vadose zone
(sometimes also
referred to as
unsaturated zone)

Critical zone

Plants
+
Vadose zone
+
Groundwater
(until bedrock)

VZ and CZ are both complex systems:

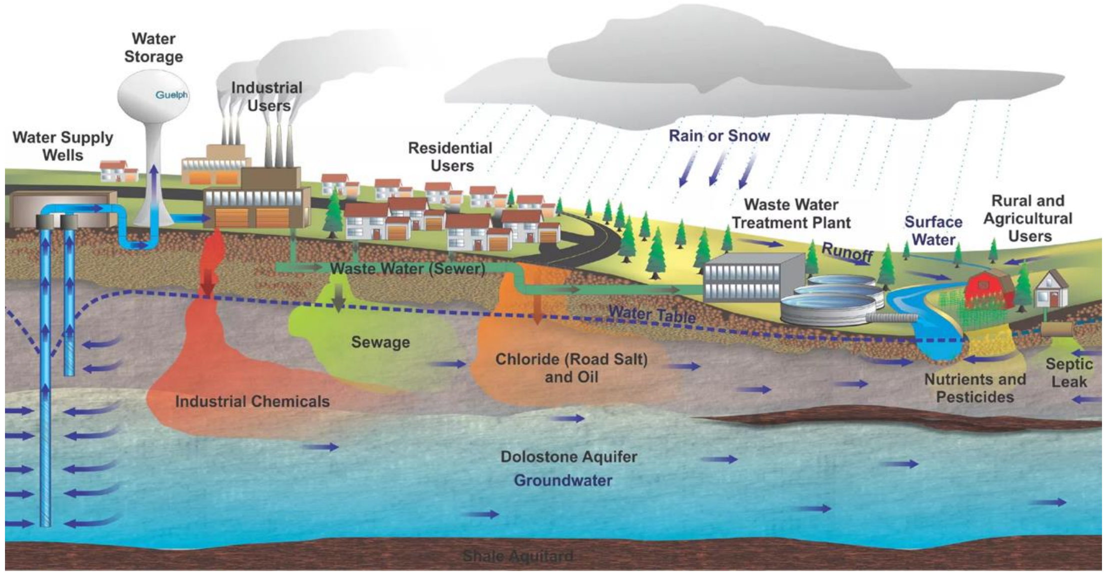
- Fluid flow processes
- Geomechanical processes
- Geochemical processes
- Microbial processes

…

Vadose Zone: Context and who cares?

Agriculture and food production

Drinking water safety



Other examples?

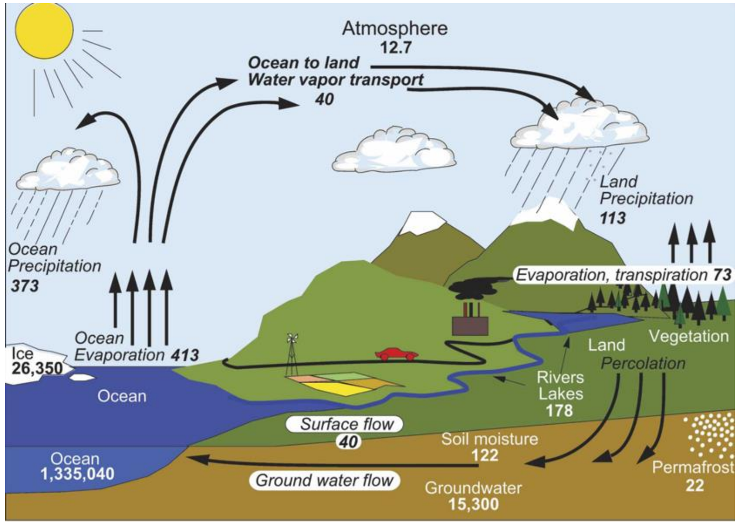
- Natural hazards management (flooding, landslide, and erosion)
- Infrastructure development (buildings, roads, bridges, …)
- …

Vadose zone processes can have profound societal impacts

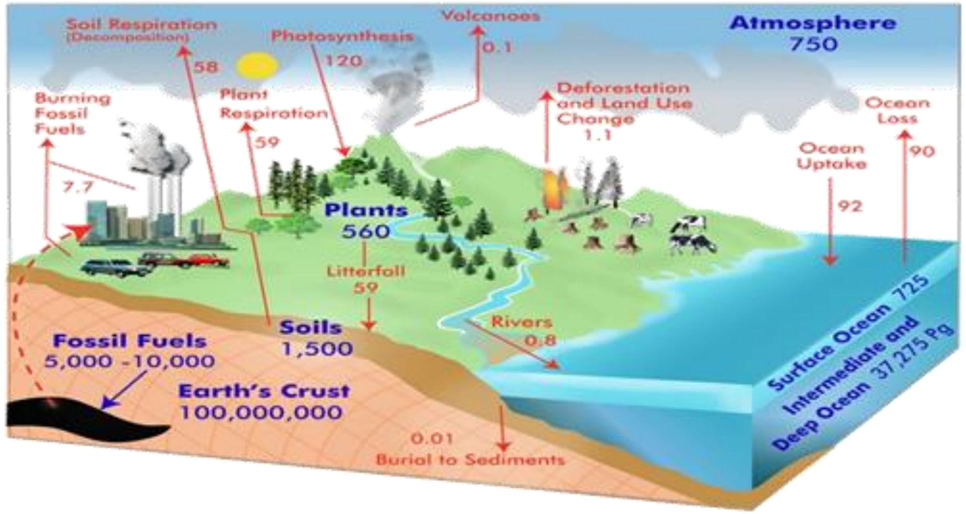
https://jooinn.com/agricultural-lands.html
https://g360group.org

Vadose Zone: Context and who cares?

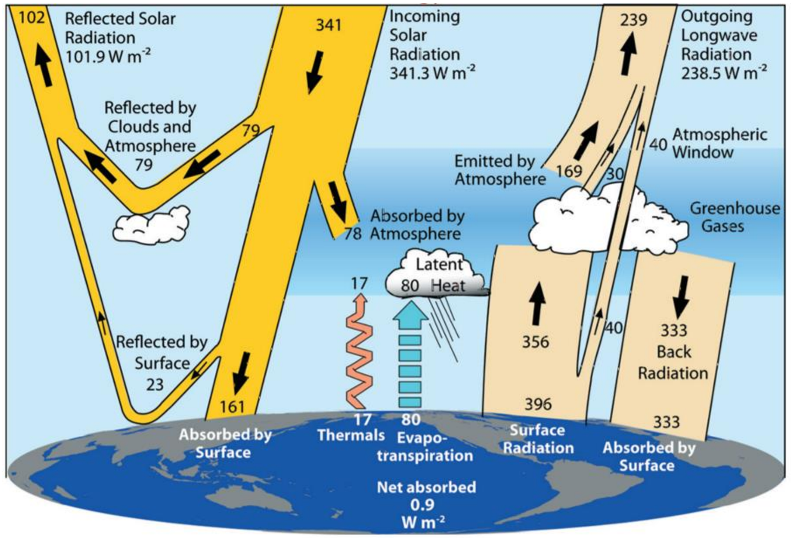
Hydrological cycle



Carbon cycle



Surface energy balance



Vadose zone processes play key roles in the global water, carbon, and energy balances

http://www.cgd.ucar.edu/cas/adai/papers/Trenberth_etal_JHM07.pdf
https://www.nasa.gov/topics/nasalife/features/globe-workshop.html
http://www.cgd.ucar.edu/staff/trenbert/trenberth.papers/BAMSmarTrenberth.pdf

Overall scope and approach

Scope

- Solute transport in saturated porous media.
- Flow and transport in the vadose zone.
- Practical applications: Pesticide, nutrient, PFAS

Approach:

- Conceptual pictures
- Physical laws and fundamental principles
- Mathematical formulations and analytical/numerical solutions
- Model vs. reality (measurements)

Philosophy:

Understanding first principles is more important than ever in an era where computational tools and artificial intelligence can obscure physical meaning. However, teaching first principles will not be effective if we focus solely on the first principles and conceptual understanding. Rather, it often requires an iterative process going from the high-level conceptual understanding to the detailed quantitative mathematical reasoning and then back again. Guided by this view, we will strike a balance between conceptual and quantitative understanding in this class.

There will be a strong emphasis on building intuition. Midterm exam is oral and will specifically test this. Final exam is written and will test your capacity to reason quantitatively.

Syllabus

Week	Monday date	Topics covered this week	Assignment due this week
1	1/12	**Field trip** – No class	
	Module 1: Solute transport in saturated media		
2	1/21	Conservative solute transport: Pore-scale controls, macroscopic formulation, governing equations, BCs, 1D Taylor-Aris dispersion	
	1/23	Conservative solute transport: Pore-scale controls, macroscopic formulation, governing equations, BCs, 1D Taylor-Aris dispersion	
3	1/26	Conservative solute transport: Analytical solutions, breakthrough curves.	
	1/28	No class (Bo traveling)	
	1/30	No class (Bo traveling)	HW 1: Solute transport 1
4	2/2	Conservative solute transport: Analytical solutions, breakthrough curves.	
	2/3 [special lecture] 9:30-11:10	Reactive solute transport: retardation, kinetic/equilibrium adsorption	
	2/4	Reactive solute transport: Analytical solutions, breakthrough curves.	
	2/6	Reactive solute transport: Analytical solutions, breakthrough curves.	HW 2: Solute transport 2
	Module 2: Pore-scale controls and macroscopic description of variably saturated flow		
5	2/9	Pore-scale fluids distribution (capillary tubes)	
	2/10 [special lecture] 9:30-10:20	Pore-scale fluids distribution (capillary tubes)	
	2/11	Pore-scale fluids distribution (advanced porous medium models)	
	2/13	No class (Bo traveling)	
6	2/16	Macroscopic descriptions of air/water distribution	
	2/18	Macroscopic descriptions of air/water distribution	
	2/20	Macroscopic descriptions of air/water distribution	HW 3: Pore-scale fluids distribution
7	2/23	Two-phase flow. Richards' assumptions; Richards' equation.	
	2/24 [special lecture] 9:30-10:20	Two-phase flow. Richards' assumptions; Richards' equation.	
	2/25	Two-phase flow. Richards' assumptions; Richards' equation.	
	2/27	No class (Bo traveling)	

Special lectures will be in Harshbarger 232.

Syllabus

Module 3: Steady-state and transient variably saturated flow			
8	3/2	Steady-state 1D unsaturated flow.	
	3/4	Steady-state 1D unsaturated flow.	
	3/6	Steady-state 1D unsaturated flow.	HW 4: Richards equation and steady-state unsaturated flow
9	3/9	No class: Spring break	
10	3/16	Steady state unsaturated flow in multiple dimensions and with heterogeneities.	
	3/18	Steady state unsaturated flow in multiple dimensions and with heterogeneities.	
	3/20	Midterm exam (oral)	
11	3/23	Transient 1D unsaturated flow. Simplified models (Green-Ampt, Philip's models).	
	3/25	Transient 1D unsaturated flow. Simplified models (Green-Ampt, Philip's models).	
	3/27	Transient 1D unsaturated flow. Simplified models (Green-Ampt, Philip's models).	HW 5: Transient unsaturated flow 1
12	3/30	Transient 1D unsaturated flow. Numerical solutions of Richards equation.	
	4/1	Transient 1D unsaturated flow. Numerical solutions of Richards equation.	
	4/2	Transient 1D unsaturated flow. Numerical solutions of Richards equation.	
13	4/6	Unsaturated flow in multidimensions.	
	4/8	Unsaturated flow in multidimensions.	
	4/10	Solute transport with unsaturated flow.	HW 6: Transient unsaturated flow 2
Module 4: Risk assessment of contaminant transport in the vadose zone and groundwater			
14	4/13	Transport of pesticides/nutrients in the vadose zone.	
	4/15	Transport of pesticides/nutrients in the vadose zone.	
	4/17	Transport of pesticides/nutrients in the vadose zone.	
15	4/20	Transport of PFAS in the vadose zone.	
	4/22	Transport of PFAS in the vadose zone.	
	4/24	Transport of PFAS in the vadose zone.	HW 7: Contaminant transport
16	4/27	Transport of PFAS in the vadose zone.	
	4/29	Transport of PFAS in the vadose zone.	
	5/1	Transport of PFAS in the vadose zone.	
17	5/4	Final exam.	

Other course information

Readings (Scan copies will be provided)

- *Contaminant Hydrogeology* — C. W. Fetter, T. Boving, and D. Kreamer (2018)
- *Subsurface Hydrology* — G. F. Pinder and M. A. Celia (2006)
- *Soil Physics* — W. A. Jury and R. Horton (2004)

Grading:

Course assignments	45%
Projects – physical hydrogeology component	10%
Midterm exam (oral)	20%
Final exam (written)	20%
Participation	5%
Art of porous media flow submission	+5%

Class websites:

1. GitHub

- https://boguoporousmedia.github.io/HWRS561b-2026Spring/
- The **primary** site that we use for sharing lecture notes and scheduling.

2. D2L

- Reading materials and materials for homework and exams.
- Submit homework and exams.

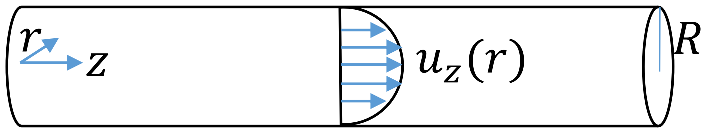
Steady-state saturated flow

$$\frac{D}{Dt} = \frac{\partial}{\partial t} + u_r\frac{\partial}{\partial r} + \frac{u_\theta}{r}\frac{\partial}{\partial \theta} + u_z\frac{\partial}{\partial z}$$

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2} + \frac{\partial^2}{\partial z^2}$$

Permeability $[L^2]$

"Hagen-Poiseuille" flow



Note for the Laplacian: $\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right)$

Navier-Stokes Equation

$$\rho\cancelto{0}{\frac{Du_z}{Dt}} = -\frac{\partial p}{\partial z} + \cancelto{0}{f_z} + \mu\nabla^2 u_z$$

Steady state & low Reynolds #

Neglect body forces

<u>Notes for Darcy's Law</u>:

$$q = -K\nabla H = -K\nabla\psi = -\frac{k\rho g}{\mu}\nabla\psi = -\frac{k}{\mu}\nabla p$$

$$K = \frac{k\rho g}{\mu}$$

$$p = \rho g\psi$$

$$\Rightarrow \mu\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial u_z}{\partial r}\right) = \frac{\partial p}{\partial z}$$

$$\frac{\partial}{\partial r}\left(r\frac{\partial u_z}{\partial r}\right) = \frac{r}{\mu}\frac{\partial p}{\partial z}$$

$$r\frac{\partial u_z}{\partial r} = \frac{r^2}{2\mu}\frac{\partial p}{\partial z} + C_1$$

$$\frac{\partial u_z}{\partial r} = \frac{r}{2\mu}\frac{\partial p}{\partial z} + \frac{1}{r}C_1$$

$$\Rightarrow u_z = \frac{r^2}{4\mu}\frac{\partial p}{\partial z} + C_1\ln r + C_2$$

BC:

$$\frac{\partial u_z}{\partial r}\Big|_{r=0} = 0 \Rightarrow C_1 = 0$$

$$u_z\big|_{r=R} = 0 \Rightarrow C_2 = -\frac{R^2}{4\mu}\frac{\partial p}{\partial z}$$

$$\Rightarrow u_z = \frac{1}{4\mu}\frac{\partial p}{\partial z}(r^2 - R^2)$$

$$Q = \int_0^R 2\pi r u_z\,\mathrm{d}r = \int_0^R \frac{\pi}{2\mu}\frac{\partial p}{\partial z}(r^3 - rR^2)\,\mathrm{d}r$$

Darcy's Law

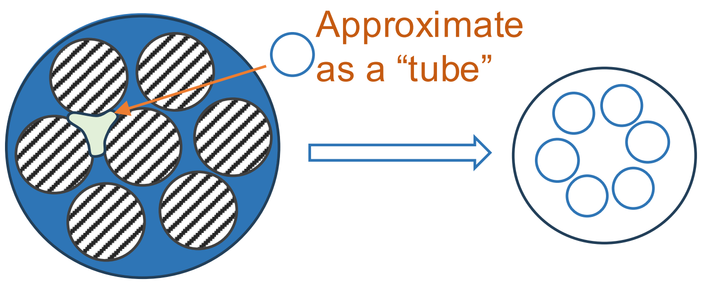
$$\Rightarrow q = \frac{Q}{A} = -\frac{R^2/8}{\mu}\frac{\partial p}{\partial z}$$

$$\Rightarrow k = R^2/8 \quad [L^2]$$

$\boxed{\text{=> The permeability of the tube is } k = R^2/8}$

Steady-state saturated flow

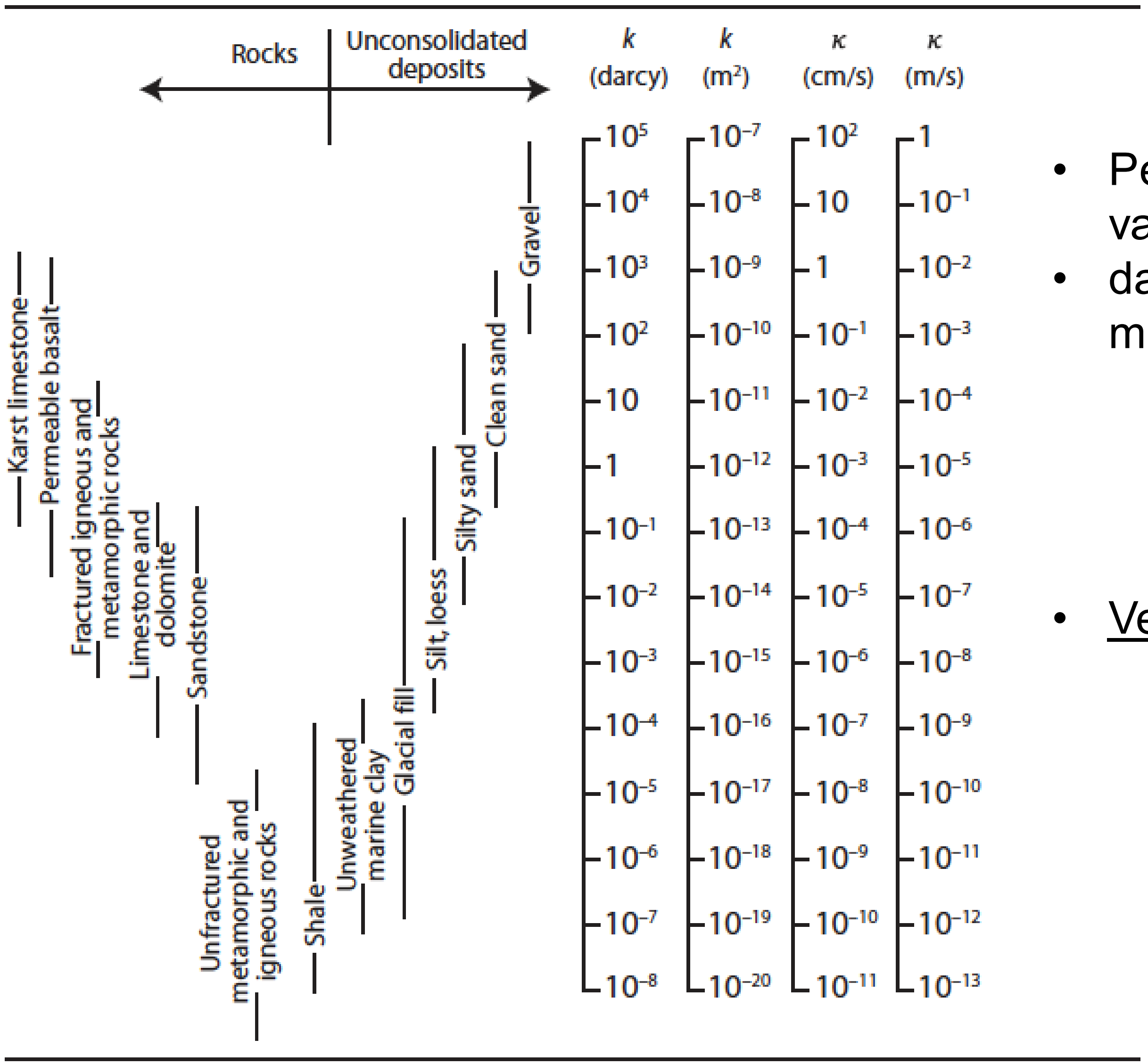
- Derivation of permeability for a tube based on the Hagen-Poiseuille flow (simplified N-S equation).
  - ✓ Permeability ~ R^2
  - ✓ The origin of Darcy's law is N-S equation
  - ✓ Permeability for a bundle of tubes of uniform size?



$$\left.\begin{matrix} n \text{ tubes} \\ k_{ST} \\ \phi \end{matrix}\right\} \Rightarrow \left.\begin{matrix} \bar{q} = \dfrac{nq\pi R^2}{n\pi R^2/\phi} = \phi q = -\phi \dfrac{k_{ST}}{\mu}\dfrac{\partial p}{\partial x} \\ \bar{q} = -\dfrac{k_{BoT}}{\mu}\dfrac{\partial p}{\partial x} \end{matrix}\right\} k_{BoT} = \phi k_{ST}$$

k_{ST} is the permeability for a single tube.

Steady-state saturated flow



(Freeze and Cherry, 1979)

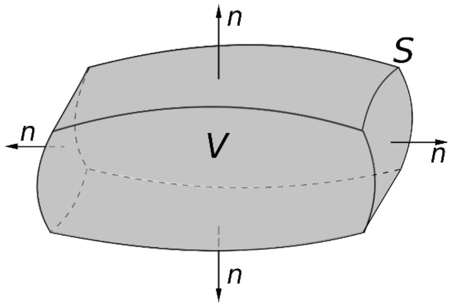
- Permeability and conductivity values for various soil and rock media
- darcy (d) = $9.869233 \times 10^{-13}\ \mathrm{m}^2 \approx 1\ \mu\mathrm{m}^2$. millidarcy (md) = 0.001 darcy.

  A porous medium with a permeability of 1 darcy permits a flow of 1 cm³/s of a fluid with viscosity 1 cP (1 mPa·s) under a pressure gradient of 1 atm/cm acting across an area of 1 cm².

  9.869233=1/1.013250. 1 atm = 1.013250 x 10^5 Pa
- Velocity of groundwater flow $\sim 1\ \mathrm{m/day}$

Steady-state saturated flow

Derive the flow equation:

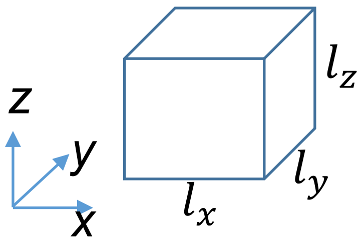


Recall: Divergence theorem

$$\int_{\partial\Omega} \boldsymbol{q} \cdot \boldsymbol{n} \, \mathrm{d}s = \int_{\Omega} \boldsymbol{\nabla} \cdot \boldsymbol{q} \, \mathrm{d}V$$

=> Divergence theorem converts a surface integral to a volume integral.

Mass conservation: Change of mass storage = mass in – mass out.



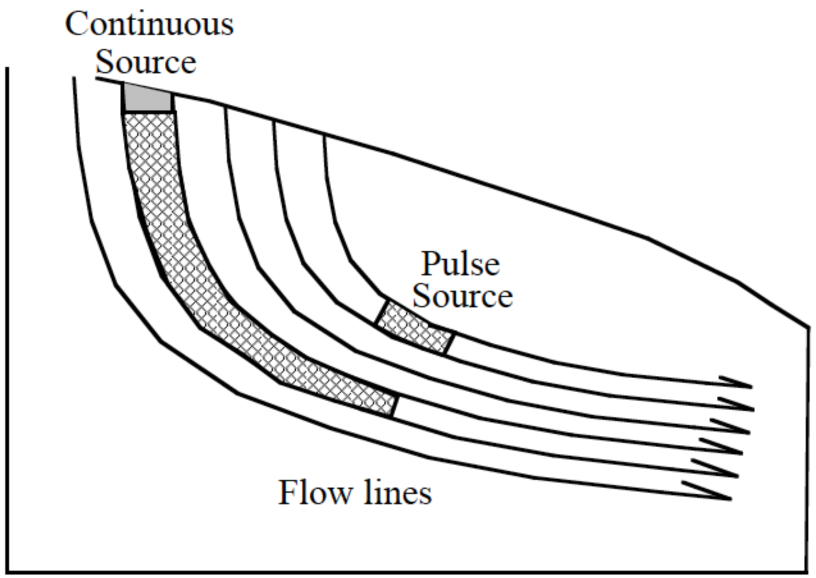
Rate of mass change:

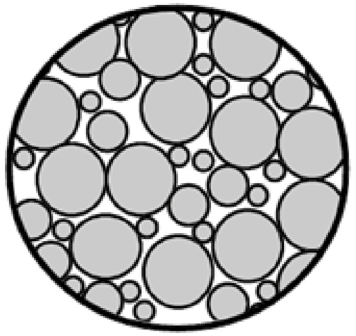
Net fluxes:

Steady-state saturated flow

Solute transport under saturated flow

Advection: The solute particles move along streamlines with a velocity equal to the groundwater velocity

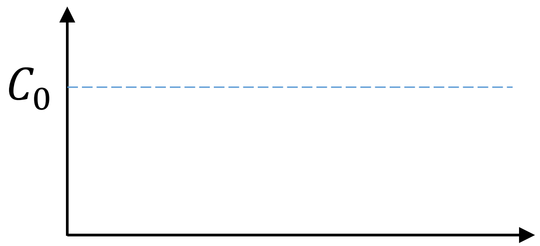




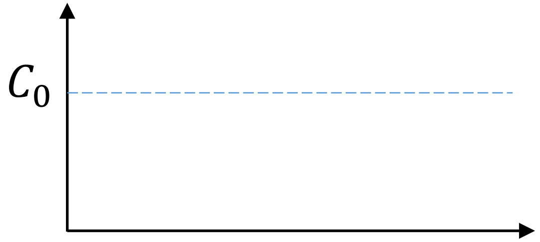
Porewater velocity is greater than the volumetric Darcy flux

Breakthrough curve (BTC)

Continuous source:



Pulse source:



Solute transport under saturated flow

Molecular diffusion: Solute particles move due to random molecular motion.

Free water: Recall Fick's Law

$$\boldsymbol{q}_c = -D_0 \boldsymbol{\nabla} \mathrm{C}.$$

Porous medium:

$$\boldsymbol{q}_c = -\phi D_d \boldsymbol{\nabla} \mathrm{C}.$$

$D_d = D_0 w$ is the effective diffusion coefficient, and w $(0 < w < 1)$ is the tortuosity factor. (Note: tortuosity vs. tortuosity factor)

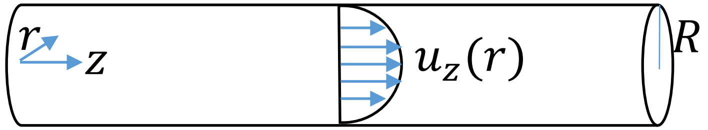
Mechanical dispersion: Mixing due to local-scale variations in groundwater velocity

Example: Dispersion in a capillary tube [G.I. Taylor (1953) and R. Aris (1956)]

Solute transport under saturated flow

Taylor-Aris Dispersion: Dispersion in a capillary tube [G.I. Taylor (1953) and R. Aris (1956)]

Solute transport in "Hagen-Poiseuille" flow



Governing equation for solute transport in the tube:

$$\frac{\partial C}{\partial t} + 2u\left[1 - \left(\frac{r}{R}\right)^2\right]\frac{\partial C}{\partial x} - D_0\left(\frac{\partial^2 C}{\partial r^2} + \frac{1}{r}\frac{\partial C}{\partial r} + \frac{\partial^2 C}{\partial x^2}\right) = 0$$

At sufficiently long times (derivation via the perturbation method)

$$\frac{\partial \bar{C}}{\partial t} + \bar{u}\frac{\partial \bar{C}}{\partial x} - D_L\frac{\partial^2 \bar{C}}{\partial x^2} = 0, \qquad D_L = D_0 + \frac{R^2\bar{u}^2}{48D_0}$$

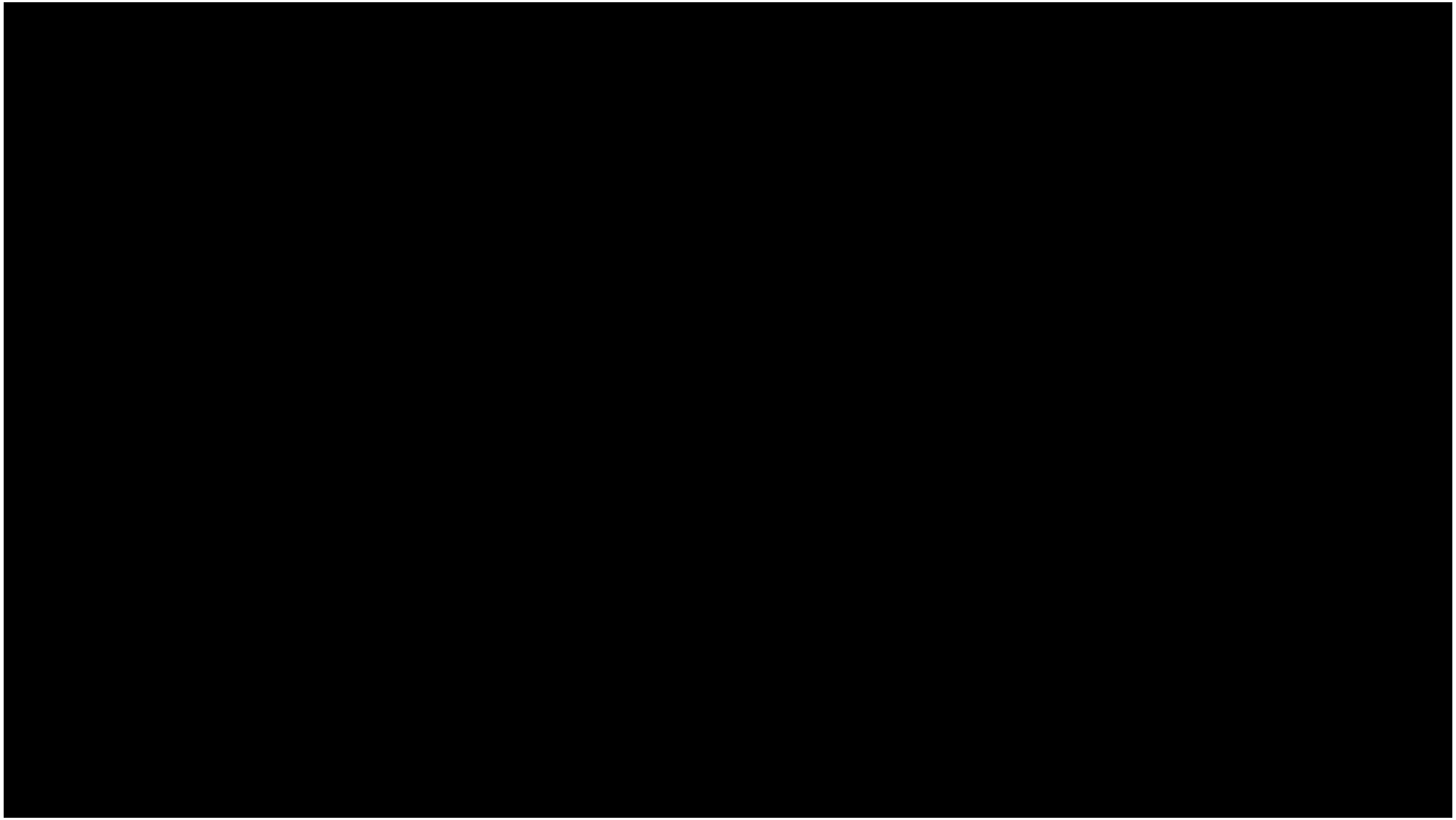
$\bar{u}$: mean velocity in the tube.
C_m: mean concentration in the tube.

$$C_m = \frac{\int_0^{2\pi}\int_0^R C(r,x)\, r\, \mathrm{d}r\, \mathrm{d}\theta}{\int_0^{2\pi}\int_0^R r\, \mathrm{d}r\, \mathrm{d}\theta} = \frac{2}{R^2}\int_0^R C\, r\, \mathrm{d}r$$

Insights: The average solute concentration spreads out by a dispersion process (radial diffusion and axial advection) and follows Fickian diffusion. The effective diffusivity is not the molecular diffusivity D_0. Rather, it is D_0 + a quadratic function of the mean velocity.

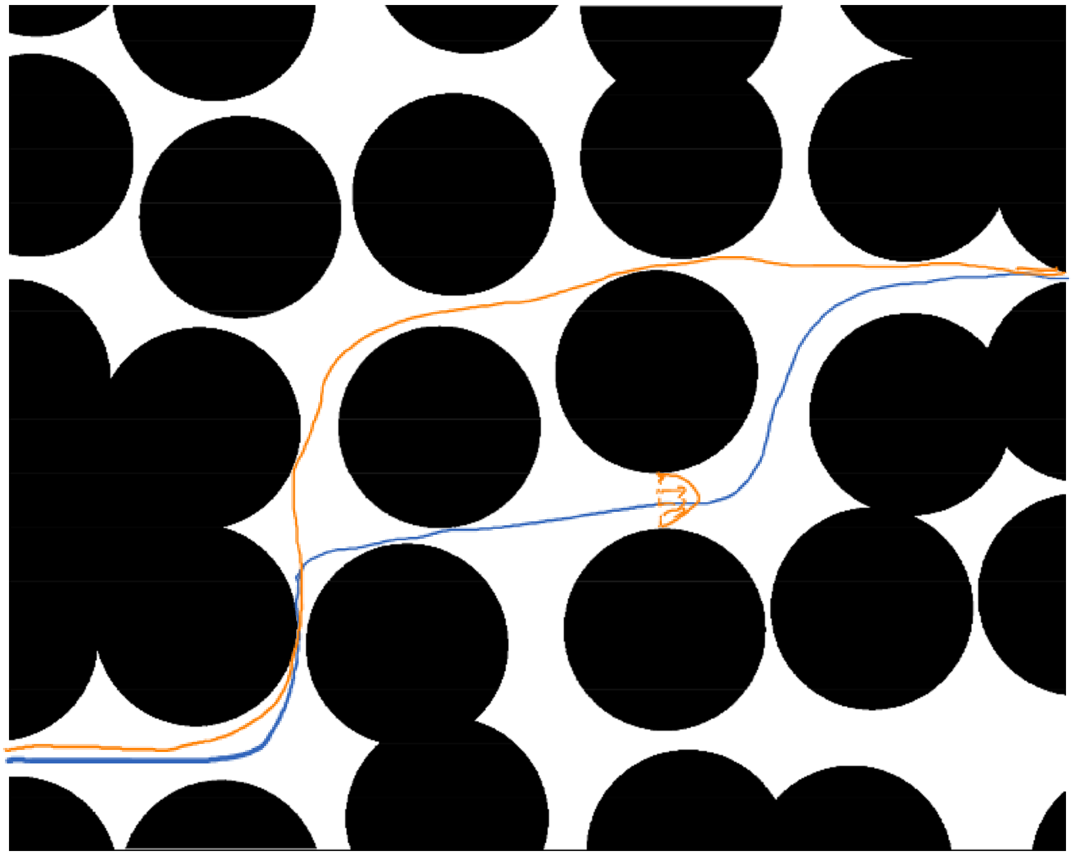
Solute transport under saturated flow

Illustrative numerical simulations of Taylor-Aris dispersion (https://youtu.be/toC4RM_aUS4)



Solute transport under saturated flow

Taylor-Aris Dispersion: Spatial variation of velocity leads to dispersion of solutes

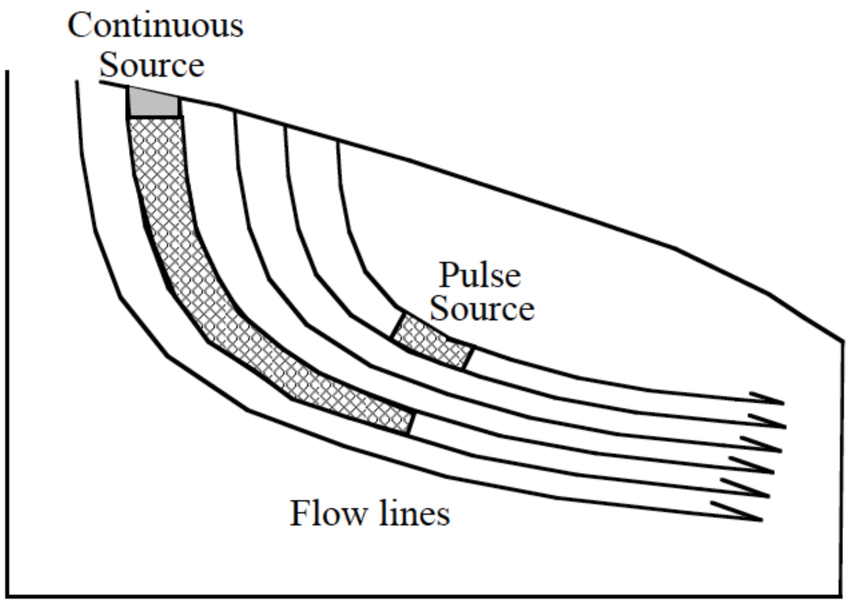


Spatial variation of velocity in a porous medium:

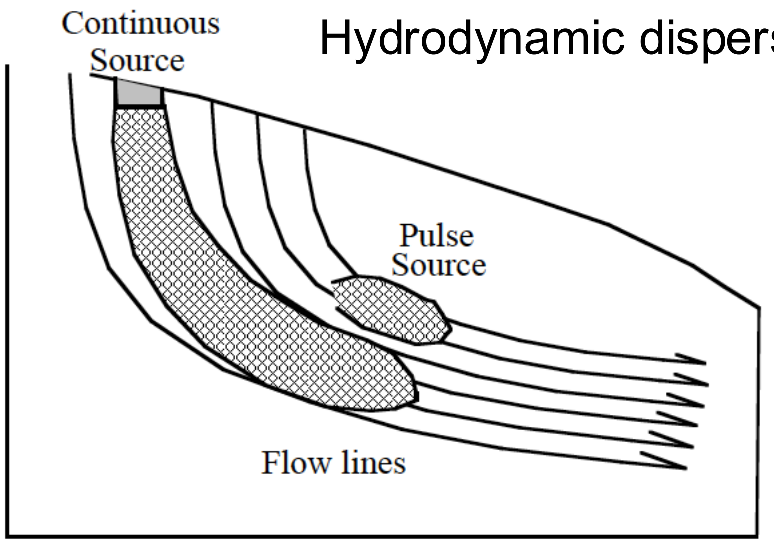
(1) Velocity profile through a pore throat (related to T-A dispersion)
(2) Velocity variation among pore throats
(3) Tortuosity

Solute transport under saturated flow

Pure advection



Advection + $\underbrace{\text{Mechanical dispersion + Molecular diffusion}}_{\text{Hydrodynamic dispersion}}$



A widely used theory for describing solute flux in saturated porous media [J. Bear (1961)]

$$\boldsymbol{q}_c = \phi(\boldsymbol{v}C - \boldsymbol{D}\nabla C),$$

- $\boldsymbol{q}_c$ is the solute flux vector.
- $\boldsymbol{v}$ is the velocity field.
- $\boldsymbol{D}$ is a tensor that depends on the velocity field and molecular diffusion in the porous medium.

For a special case in 1D flow:

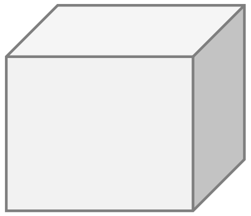
$$D_{xx} = \alpha_L v_x + D_d$$

$$D_{yy} = D_{zz} = \alpha_T v_x + D_d$$

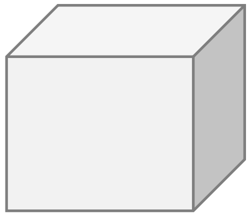
- α_L and α_T are longitudinal and transverse dispersivities, respectively.

Solute transport under saturated flow

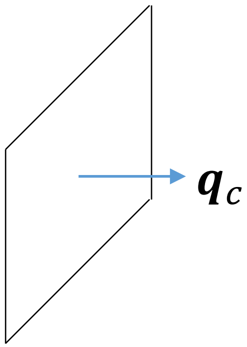
HWRS 561b
Bo Guo
Spring 2026

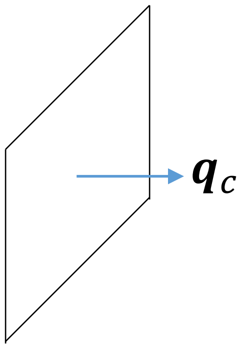


Saturated
porous medium



Fluid only
(e.g., free water)



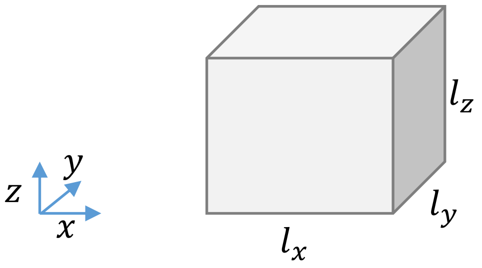


$$\begin{aligned}\boldsymbol{q}_c &= \phi(\boldsymbol{v}C - \boldsymbol{D}\nabla C)\\ &= \boldsymbol{q}C - \phi\boldsymbol{D}\nabla C\end{aligned}$$

$$\boldsymbol{D} = \alpha_T|\boldsymbol{v}|\mathbf{I} + (\alpha_L - \alpha_T)\frac{\boldsymbol{v}\boldsymbol{v}}{|\boldsymbol{v}|} + wD_0\mathbf{I}$$

$$\boldsymbol{q}_c = \boldsymbol{v}C - D_0\nabla C$$

Solute transport under saturated flow



$$C(x, y, z, t) = \frac{\text{mass of solute}}{\text{unit fluid volume}}$$

Mass conservation: Change of mass storage = mass in – mass out.

Rate of mass change:

Net fluxes:

Solute transport under saturated flow