Numerical Simulation of Transport Processes in Porous Media

Introduction

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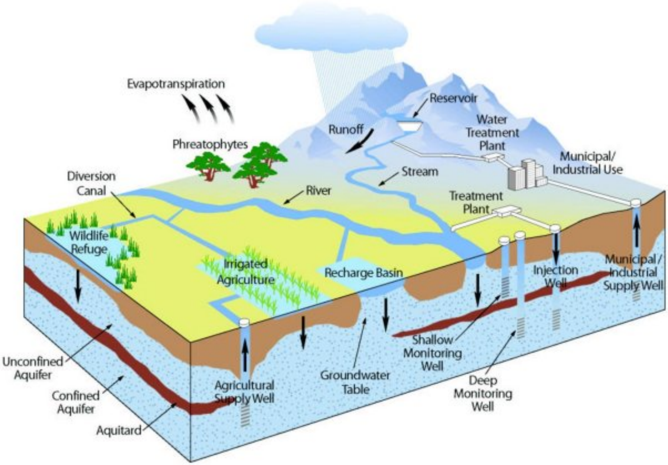
Groundwater Production



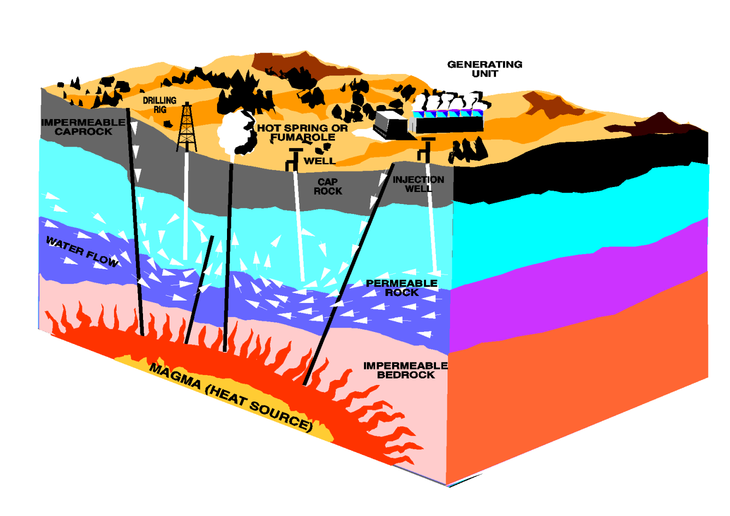
from: V. M. Ponce: Sustainable Yield of Ground Water (`http://ponce.sdsu.edu/groundwater_sustainable_yield.html`)

Agriculture

from: Wikipedia Commons, Author: Myrabella

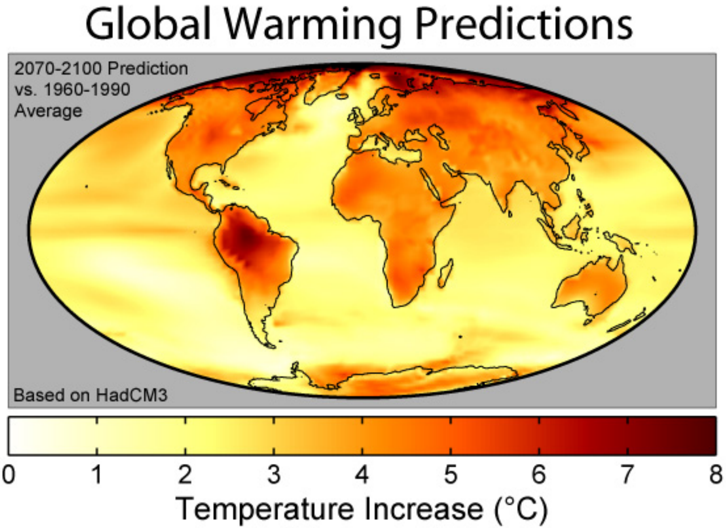
Contaminated Sites and Remediation

Geothermal Energy



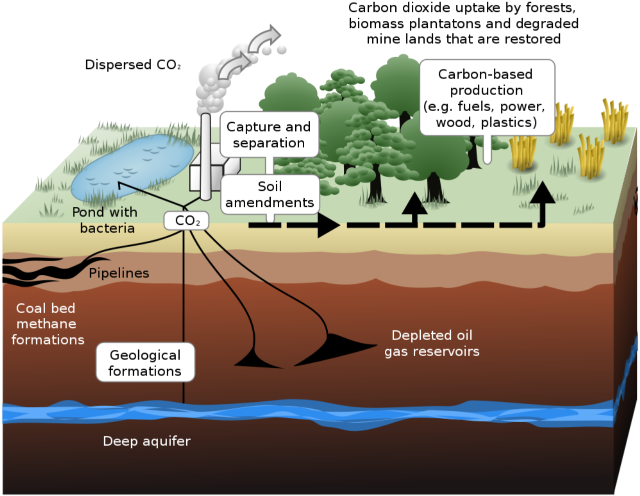
from: Energy Information Administration, Geothermal Energy in the Western United States and Hawaii: Resources and Projected Electricity Generation Supplies, DOE/EIA-0544 (Washington, DC, September 1991
(`http://www.eia.doe.gov/cneaf/solar.renewables/renewable.energy.annual/backgrnd/fig19.htm`)

Global Climate Prediction, Reconstruction of Paleo-Climate



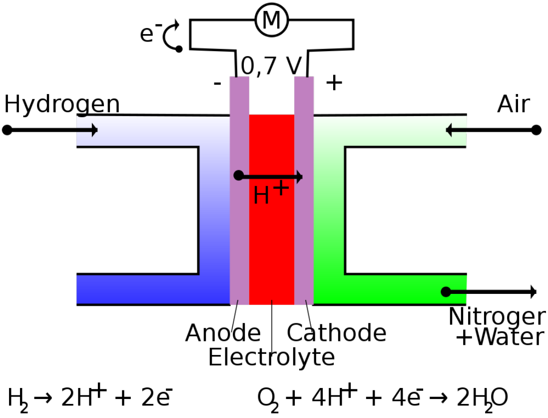
from: Wikipedia Commons, Author: Robert A. Rohde for Global Warming Art (`http://www.globalwarmingart.com/`)

Carbon Dioxide Sequestration



from: Wikipedia Commons, Authors: LeJean Hardin and Jamie Payne
(`http://http://www.ornl.gov/info/ornlreview/v33_2_00/research.htm`)

Catalyst Research, Fuel Cells



from: Wikipedia Commons, Author: HandigeHarry

Transport in Brain Tissue

from: Wikipedia Commons, Author: Woutergroen

Intention of the Lecture

- Introduction to the physics of transport in porous media
- Learning the necessary basics on
  - Discretisation of partial differential equations, in particular the Finite-Volume method
  - Iterative solution of linear equation systems
  - Time discretisation
  - Solution of non-linear partial differential equations
  - Bottom-up implementation of numeric solvers
- Aims:
  - Get an insight in the operation of simulation programs
  - Get a better understanding for the behaviour of existing solvers for partial differential equations
  - Get a better understanding for the possible phenomena occuring in porous media flow

Prerequisites

For the lecture

- Basic knowledge of numerical mathematics
- Basic knowledge about partial differential equations

For the exercises

- Basic knowledge of object-oriented programming with C++ (Info1 lecture)
- Readiness to do some programming in the exercises

Topics

- Classification of partial differential equations
- Spatial discretization methods
- Finite-Volumen methods
- Iterative solvers
- Groundwater flow / elliptic PDE
- Heat conduction / parabolic PDE
- Solute transport / hyperbolic PDE
    - Particle Tracking
    - Higher-order methods
    - Solute sorption
- Solution of non-linear equations
- Water transport in unsaturated porous media

Exercises

- The exercises are a crucial part of the lecture
- You understand a numerical algorithm best if you have implemented it once
- The implementation is done bit by bit without use of external libraries

Script and Webpage

There is a course webpage at

http://conan.iwr.uni-heidelberg.de/teaching/numpormed_ws2009/index_e.html

You can find there

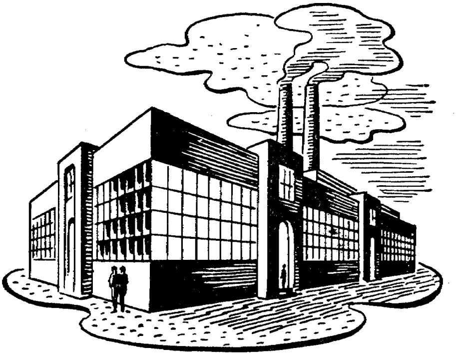
- the transparencies of the lectures
- a script for the course
- the exercise sheets
- sample solutions (after the discussion of the exercise)

Groundwater contamination problem

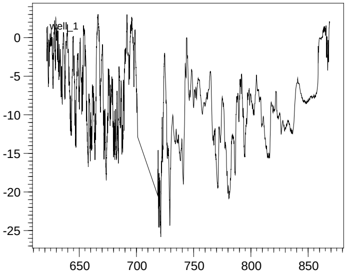
The water in several wells is contaminated with a soluble substance.

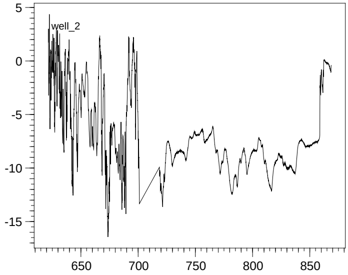
Groundwater contamination problem

We know that there was an accident in a factory where the same substance was released to the groundwater.



Groundwater contamination problem



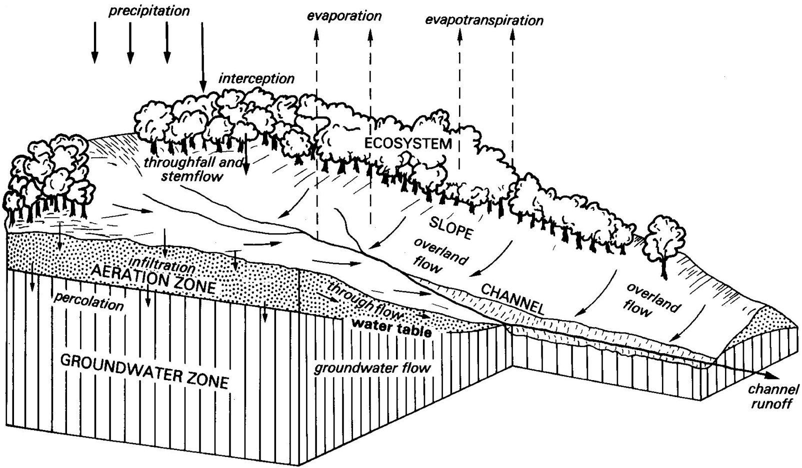


- Does this explain all the contamination?
- Can we reproduce the measurements?
- Is there another source involved?

What do we have to do to solve this problem?

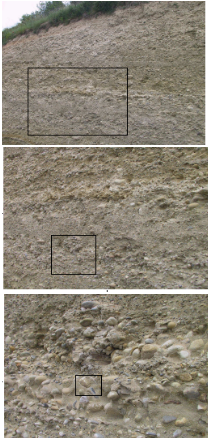
- Compute the flow field for groundwater
- Determine the amount of contamination from the factory
- Solve solute transport problem
- Compare measurements at wells with the result

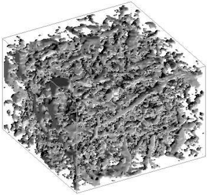
Groundwater Flow

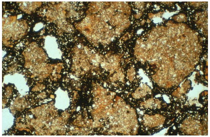


from: Environmental Systems - An introductory text, I. D. White, D. N. Mottershead, S. J. Harrison, 2nd edition, Chapman & Hall

Heterogeneity





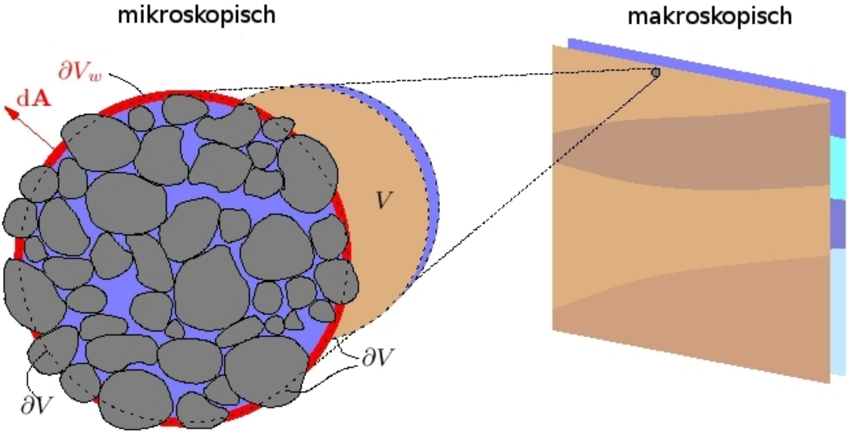


from: K. Roth (2005), Soil Physics - Lecture Notes v1.0, Institut für Umweltphysik, Universität Heidelberg
http://www.iup.uni-heidelberg.de/institut/forschung/groups/ts/students/lecture_notes05/lecture_notes05.html

Anisotropy

from: K. Roth (2005), Soil Physics - Lecture Notes v1.0, Institut für Umweltphysik, Universität Heidelberg
http://www.iup.uni-heidelberg.de/institut/forschung/groups/ts/students/lecture_notes05/lecture_notes05.html

Continuum approach



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http://www.iup.uni-heidelberg.de/institut/forschung/groups/ts/students/lecture_notes05/lecture_notes05.html

Darcy Equation

H. Darcy (1856): Les Fontaines de la Ville de Dijon, Dalmont, Paris.

$$J_w = -K_s \cdot \frac{\Delta p_w}{\Delta x}$$

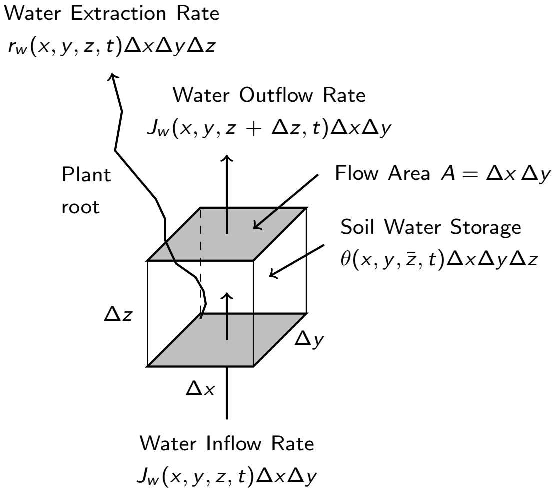
for $\Delta x \rightarrow 0$

$$J_w = -K_s \cdot \frac{\partial p_w}{\partial x}$$

in three dimensions:

$$\vec{J}_w = -\bar{K}_s \cdot \begin{pmatrix} \frac{\partial p_w}{\partial x} \\ \frac{\partial p_w}{\partial y} \\ \frac{\partial p_w}{\partial z} \end{pmatrix} = -\bar{K}_s \cdot \nabla p_w$$

Mass Conservation



according to W. A. Jury, R. Horton (2004): Soil Physics, 6th ed, Wiley & Sons, New Jersey

Transport Equation

$$
\begin{aligned}
\frac{\partial\theta(\vec{x})}{\partial t} + \nabla \cdot \vec{J}_w(\vec{x}) + r_w(\vec{x}) &= 0 \\
\frac{\partial\theta(\vec{x})}{\partial t} + \nabla \cdot \left[-\bar{K}_s(\vec{x}) \cdot \nabla p_w\right] + r_w(\vec{x}) &= 0 \\
\frac{\partial\theta(\vec{x})}{\partial t} - \nabla \cdot \left[\bar{K}_s(\vec{x}) \cdot \nabla p_w\right] + r_w(\vec{x}) &= 0
\end{aligned}
$$

with gravity:

$$
\frac{\partial\theta(\vec{x})}{\partial t} - \nabla \cdot \left[\bar{K}_s(\vec{x}) \cdot (\nabla p_w - \rho_w g \vec{e}_z)\right] + r_w(\vec{x}) = 0
$$

Steady-State:

$$
-\nabla \cdot \left[\bar{K}_s(\vec{x}) \cdot (\nabla p_w - \rho_w g \vec{e}_z)\right] + r_w(\vec{x}) = 0
$$

Summary: Groundwater Flow

- Groundwater flow can be described by Darcy's Law $J_w = -K_s \nabla p_w$ and the continuity equation $\frac{\partial \theta(\vec{x})}{\partial t} + \nabla \cdot \vec{J}_w(\vec{x}) + r_w(\vec{x}) = 0$.
- Gravity results in an addition driving force $-\rho_w g \vec{e}_z$:

$$\frac{\partial \theta(\vec{x})}{\partial t} - \nabla \cdot \left[\bar{K}_s(\vec{x}) \cdot (\nabla p_w - \rho_w g \vec{e}_z)\right] + r_w(\vec{x}) = 0$$

- Heterogeneity is considered by different values of K_s at different positions of $\vec{x}$
- Anisotropy is considered by using a tensor $\bar{K}_s$ instead of a scalar
- In steady state the flux equation is given by:

$$-\nabla \cdot \left[\bar{K}_s(\vec{x}) \cdot (\nabla p_w - \rho_w g \vec{e}_z)\right] + r_w(\vec{x}) = 0$$