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Evaluation of different modeling approaches to simulate contaminant transport in a fractured limestone aquifer

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Introduction and objectives

It is important to understand the fate and transport of contaminants in limestone aquifers because they are a major drinking water resource in Denmark.

Several modeling approaches have been developed to describe solute transport in fractured media. However, these modeling concepts are not well tested for fractured limestone geologies.

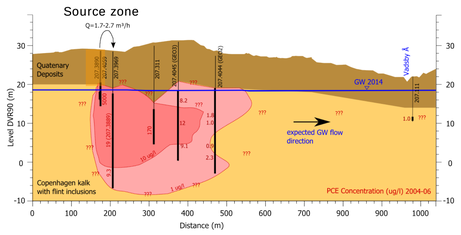
The objective is to develop the modeling tools that are needed to simulate contaminant transport in fractured limestone aquifers

- Improve risk assessment and remediation design
- Provide knowledge of the processes affecting the field scale behavior of contaminant plumes, e.g. fracture flow and back diffusion from the matrix
- Provide the means to interpret lab and field data
- Provide input to experimental and monitoring design

→ Tight coupling between modeling and field work

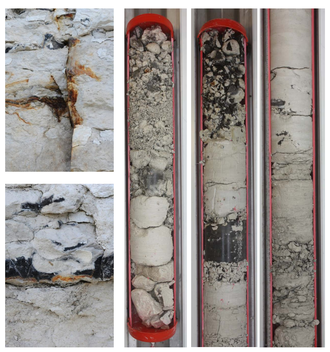
Site description

- Contaminated site in Denmark: PCE spill in the 1970s (dry cleaner facility)
- Excavation of most contaminated area in 2006
- Installation of pump-and-treat system
- Currently: new measurements and new monitoring boreholes



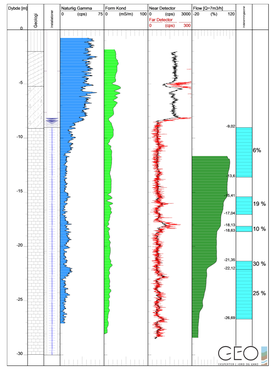
Geology

- Strongly heterogeneous
- Fractured limestone
- Flint inclusions



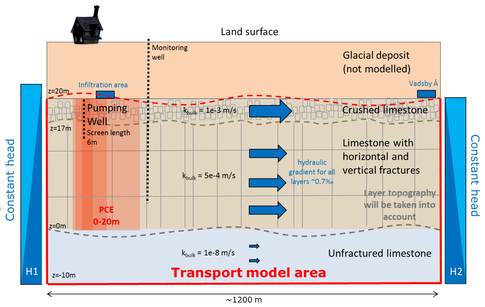
Data and measurements

- Borehole logs, groundwater potentials
- Cores from boreholes
- Pump and slug tests
- Multilevel sampling of GW for contaminant analysis
- Fracture data from outcrops and boreholes
- Existing data (e.g. reports)

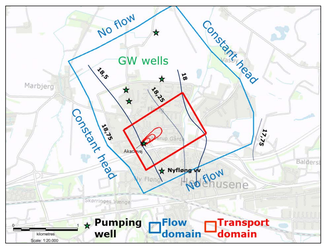


Conceptual model

Cross section



Top view



Numerical Models

DFM

Detailed model to determine parameters and validity of simplified models
Resolved fracture network and matrix
Very high computational effort

EPM

Simple approach with averaged parameters
Fractures not resolved
No back-diffusion possible
Lowest computational effort

Field data and measure-ments

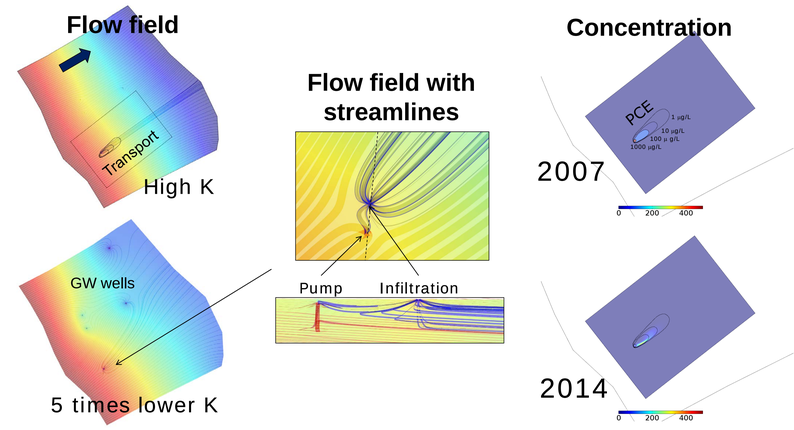
DP

Interaction between fractures and matrix by dual-porosity concept
Exchange coefficients from DFM
Back-diffusion can be described
Moderate computational effort

Why is this challenging?

- High spatial variability, difficult to acquire aquifer parameters on right scale
- Complex geology and geometry has to be integrated in model
- Little knowledge of contaminant distribution
- Concentrations from water sampling represent high-conductive zones (fractures), concentrations from fractures and matrix required
- 3D modeling to analyze transport behavior (dispersion, fracture flow)
- High conductivity contrast between fractures, limestone and flint → very fine grid required for DFM
- Stability of numerical solution
- Determination of effective parameters (conductivity, porosity, dispersivity etc.) for EPM and DP models

Preliminary modeling results – EPM



Current and future work

- 3D EPM implemented in Comsol Multiphysics with nested domains
- Flow field includes important features in the domain
- Smaller transport domain to reduce computational effort
- Modeling used for experimental and monitoring design
- Comparison with field data and model evaluation

Future work

- Integration of new measurements (e.g. flow logs)
- 3D DFM simulations with representative fracture network in part of the domain to determine parameters for EPM / dual porosity model
- Testing and comparison of currently used models for their applicability and limitations to describe contaminant transport in fractured limestone aquifers
- Testing and comparison of different modeling tools
- Analysis of plume behavior, remediation efficiency and alternatives