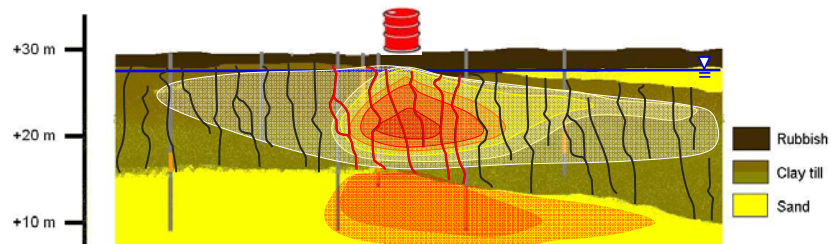


# Modeling Multi-Component Transport and Enhanced Anaerobic Dechlorination in a Single Fracture – Clay Matrix System

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## Background

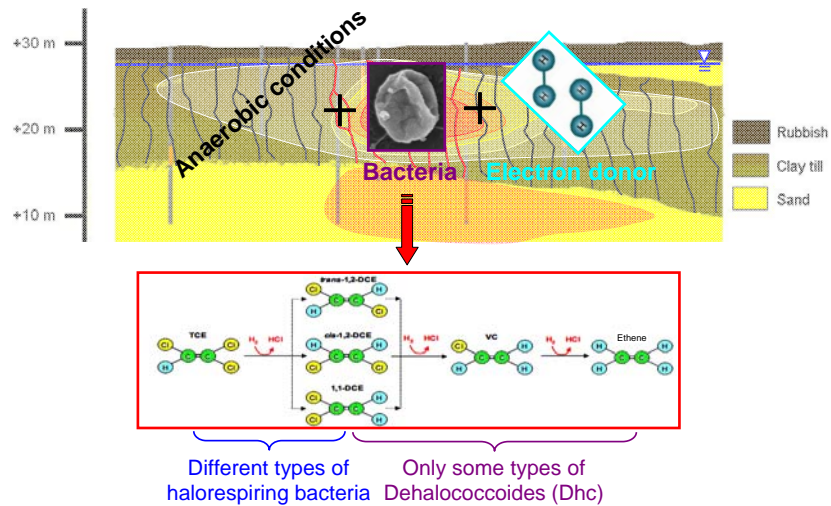
Control of source spreading and fate



# Background



## Anaerobic dechlorination



# Objectives

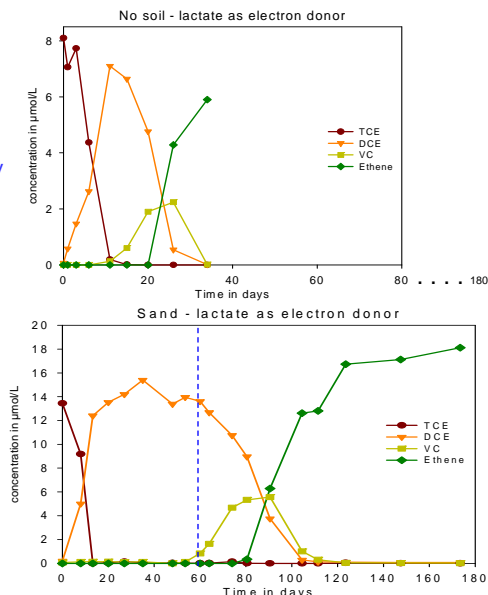


- Combine fracture/matrix model with chlorinated hydrocarbon degradation
- Different diffusion and sorption properties for the compounds
- Study where degradation takes place in fractured clay till
- Assessment of contaminant flux from fractured clays
- Perspectives for reductive anaerobic dechlorination
  - Clean-up times for fractured clay systems

# Anaerobic dechlorination



- Monod kinetics model
- Two sets of experiments
  - No soil
  - Sand from a field site (treatability study)
- Same bacteria culture KB-1™
- Two electron donors
  - Lactate (fast hydrogen releaser)
  - Propionate (slow hydrogen releaser)

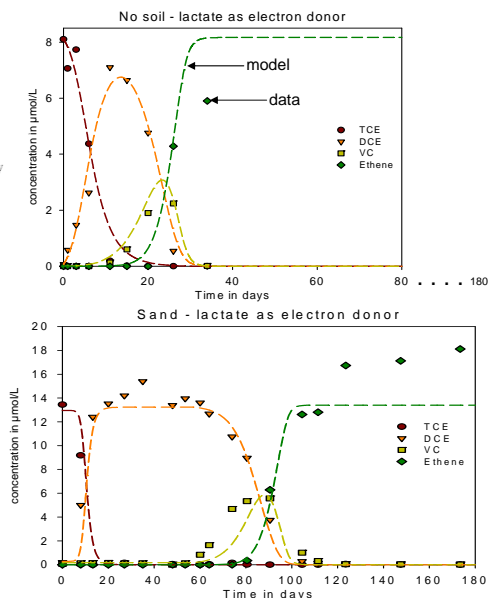


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# Anaerobic dechlorination - data



- Monod kinetics model
- Two sets of experiments
  - No soil
  - Sand from a field site (treatability study)
- Same bacteria culture KB-1™
- Two electron donors
  - Lactate (fast hydrogen releaser)
  - Propionate (slow hydrogen releaser)
- Optimization of most sensitive parameters (lactate, no soil)
  - Use of the same parameters for the experiments with sand and GW



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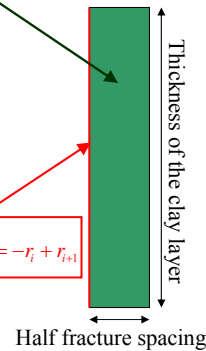
## Single fracture model - equations



- Conceptual model based on Sudicky and Frind, 1982
- Symmetry in geometry
  - Half matrix and half fracture
- Transport equations
  - Diffusion/Sorption
  - Advection/Dispersion
- Coupling fracture/matrix
  - Concentration continuity
  - Flux  $Q_m = -\phi_m D_m \frac{\partial C_m}{\partial z}$

$$R_{m,i} \frac{\partial C_{m,i}}{\partial t} = D_{m,i} \left( \frac{\partial^2 C_{m,i}}{\partial x^2} + \frac{\partial^2 C_{m,i}}{\partial z^2} \right) - r_i + r_{i+1}$$

$$\frac{\partial C_{f,i}}{\partial t} + v_f \frac{\partial C_{f,i}}{\partial z} - D_{f,i} \frac{\partial^2 C_{f,i}}{\partial z^2} + \frac{Q_m}{b} = -r_i + r_{i+1}$$



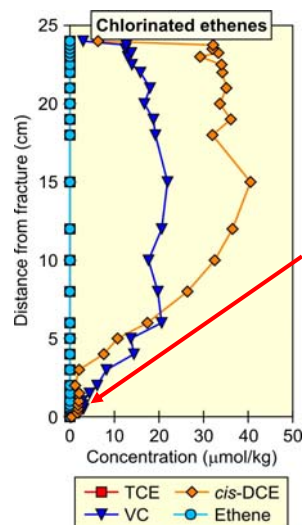
## Single fracture model - dechlorination



- Monod kinetics with previous parameters
  - Constant biomass
- Degradation location
  - Fracture
  - Matrix?
  - From literature and field data, reaction zone is limited at the fracture – clay interface



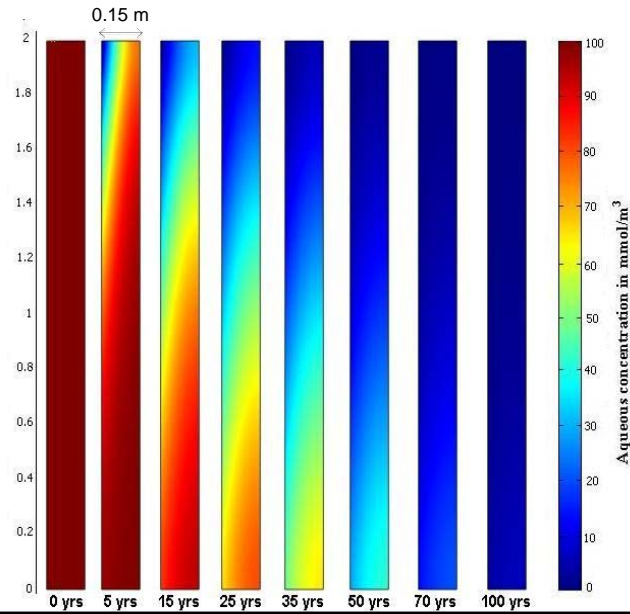
fracture



## Single fracture model - outputs



- Contaminant distribution in the matrix

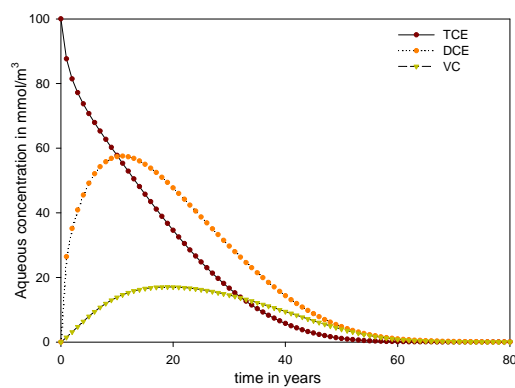


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## Single fracture model - outputs



- Contaminant distribution in the matrix
- Contaminant concentration at the fracture outlet



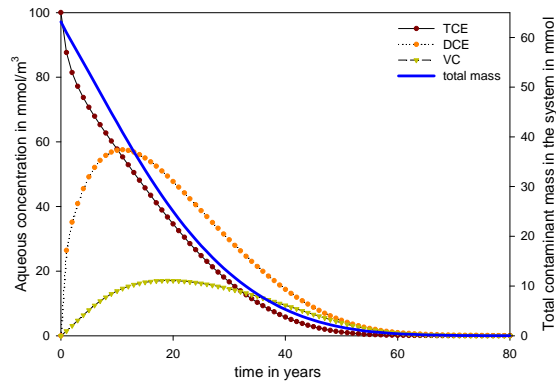
Fracture outlet

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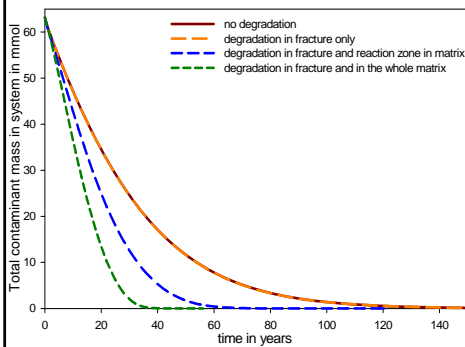
# Single fracture model - outputs



- Contaminant distribution in the matrix
- Contaminant concentration at the fracture outlet
- Total mass of contaminant in the system

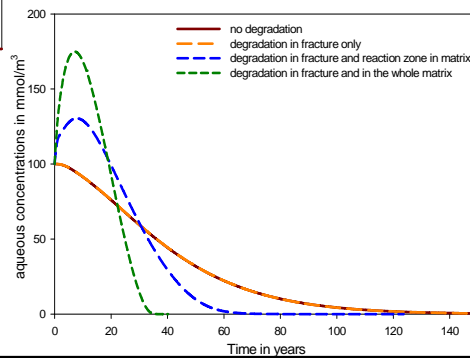


# Different degradation scenarios

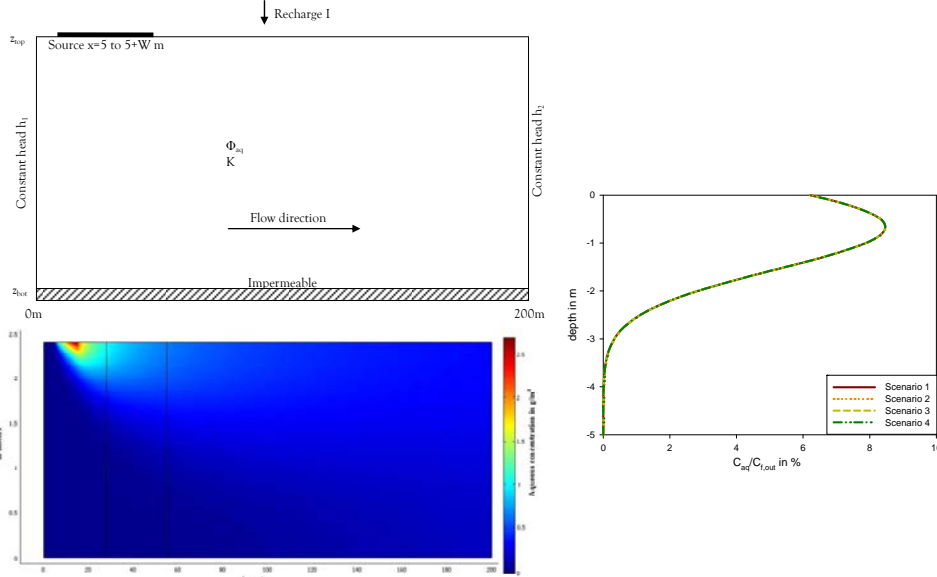


Total mass of contaminant

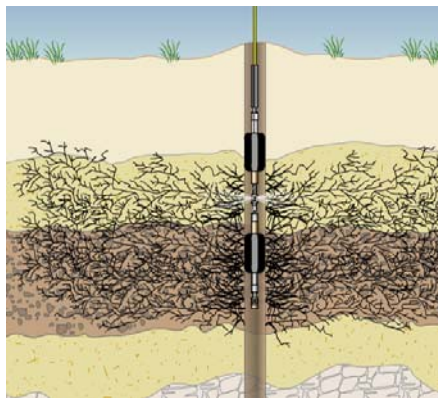
TCE, DCE, VC at the fracture outlet



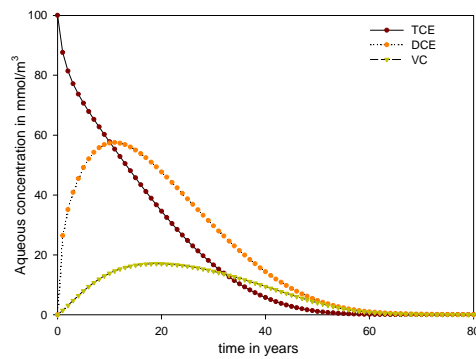
# Coupling to underlying aquifer



# Remediation perspectives



Pneumatic fracturing



→ Reduce clean-up times

## Conclusions - Perspectives



- Single fracture – matrix model combined with complex dechlorination model
  - Clean-up times
- Improvement of the dechlorination model
  - Biomass growth
  - Limiting substrate
  - Fermentation process
- Improvement of the geometry
  - Horizontal fractures
  - Heterogeneous fracture networks
- Simulation of enhanced bioremediation system design