Groundwater flow and reactive transport modelling for a quantitative assessment of natural abiotic degradation of 1.1.1-trichloroethane in a Belgian chalky aquifer

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Background

- Important chalk aquifer mainly used for drinking water.
- Local pollution with CAHs dominated by 1.1.1-TCA.
- Abiotic degradation of 1.1.1-TCA by Hydrolysis and Dehydrohalogenation (Results of Compound-Specific Isotope Analysis).
- Mineralization changes: from degradation reactions and leaching od inorganic compounds from the backfill layer.
- Parameters of the chalk formation :
  - Hydraulic conductivity : between 3×10^{-6} and 3×10^{-4} m/s.
  - Effective (transport) porosity ne: between 1 and 2%.

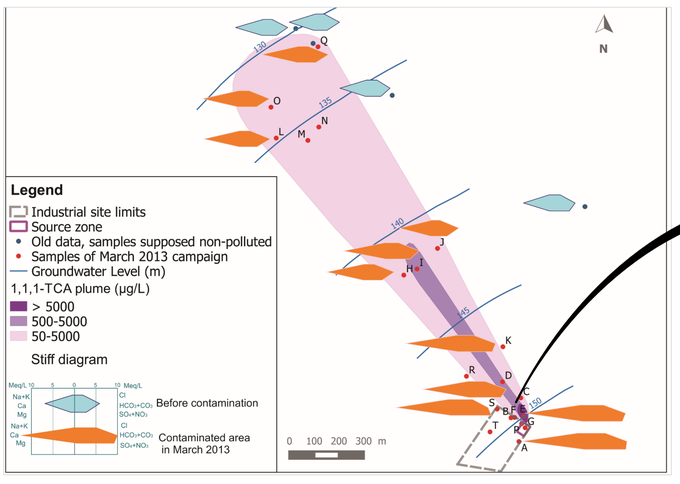

Figure 1. Stiff diagrams for groundwater samples: comparison between the contaminated area and the groundwater quality before contamination.

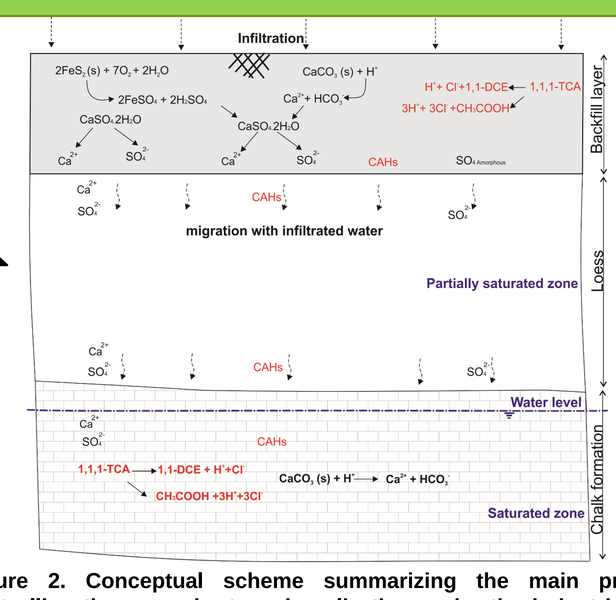

Figure 2. Conceptual scheme summarizing the main process controlling the groundwater mineralization under the industrial site. (article under review)

Objectives

Carry out a quantitative assessment of the natural attenuation processes of 1.1.1-TCA in the chalk aquifer considering mass transport processes with degradation reactions.

Methodology

Flow model

Conservative transport model

Reactive transport model

- Numerical modeling of groundwater flow and reactive transport of solute using FEFLOW®.
- Use the collected data form characterization stage and from previous studies.

Flow Model

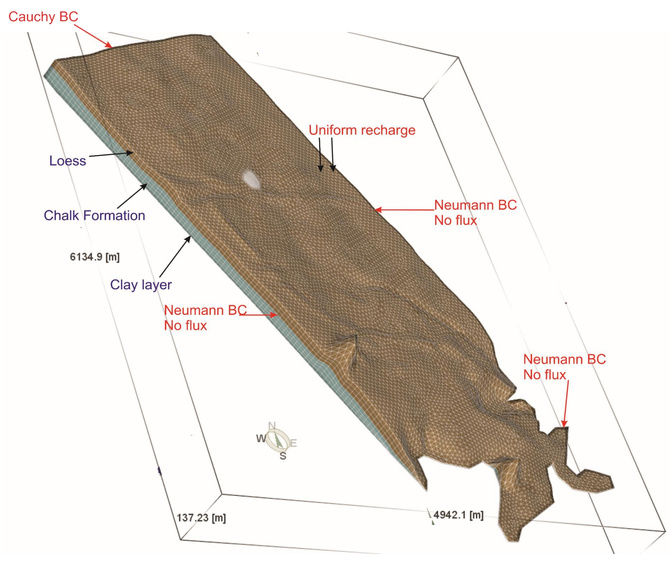

Figure 3. Boundary conditions and spatial discretization.

- Steady state saturated-unsaturated flow model.
- Equivalent hydraulic conductivity for the fissured chalk.
- Calibration with two K_h values for the chalk.
- Average annual recharge: 220 mm/an.
- Van Genuchten parameters for unsaturated flow:

	θ_s	θ_r	$\alpha(m^{-1})$	n
Loess	0.45	0.055	2	0.82
Chalk	0.41	0.055	0.16	2.42

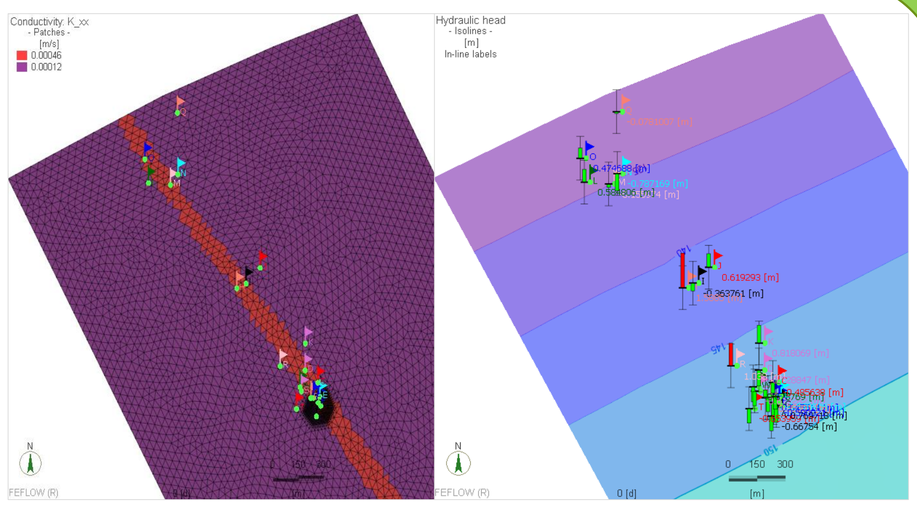

Figure 4. Hydraulic conductivity and calibration results.

Conservative transport model

- Form the site investigation results, sulphate is considered as a conservative tracer in the transport model.
- Neumann mass transport boundary conditions:
  - Source in the backfill layer,
  - Maintaining the sulphate concentration in the aquifer.
- Calibration parameters: Effective porosity, longitudinal, transverse dispersivity and molecular diffusion coefficient.

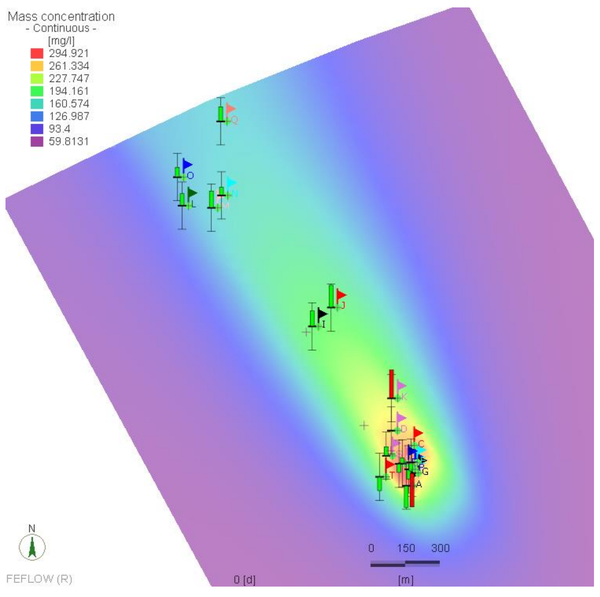

Figure 5. Simulated SO_4 plume and calibration results.

- The calibrated model is able to reproduce the observed plume with a target ± 0,6 mmol/L.
- **Calibration parameters for the chalk:**
  - Effective porosity: 2%,
  - Longitudinal dispersivity: 280 m,
  - Diffusion coefficient 3×10^{-8} m²/s.

Next steps

- Calibrate the multi-species reactive transport model considering the occurring reactions (mainly Hydrolysis and Dehydrohalogenation of 1,1,1-TCA with calcite dissolution in the chalk matrix) using observed concentrations.
- Improve the calibration with $\delta^{13}C$ and $\delta^{37}Cl$ of 1,1,1-TCA.
- The model will provide a more accurate assessment of natural attenuation process of 1,1,1-TCA in the chalk aquifer.