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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In a Belgian chalky aquifer, groundwater quality has been locally affected by a mixture of Chlorinated Aliphatic Hydrocarbons (CAHs) dominated by 1,1,1-trichloroethene (1,1,1-TCA). In a first phase, the characterization and pollution monitoring enabled the acquisition of different data, including in situ parameters, major ions, and $\delta^{13}C$ with $\delta^{37}C$ of 1,1,1-TCA. Results showed that the latter undergoes abiotic degradation by hydrolysis and dehydrohalogenation in the saturated zone affecting also the hydrochemistry in this aquifer.

The aim of our study is to carry out a quantitative assessment of the occurring natural attenuation processes of 1,1,1-TCA in the chalky aquifer by considering, in addition to mass transport processes, the observed degradation reactions and their impact on the groundwater hydrochemistry.

First, a plume-scale groundwater flow and solute transport model was built using FEFLOW (Finite Element Subsurface Flow and Transport Simulation System) considering advection and dispersion of a conservative solute. The fissured chalk was modelled as an equivalent porous medium with hydraulic conductivity and dispersivity values deduced from field data (pumping and tracer tests) of previous studies in this aquifer. Second, the occurring reactions (mainly hydrolysis and dehydrohalogenation of 1,1,1-TCA with calcite dissolution in the chalk matrix) were modelled using the piChem plugin that couples the advanced program for simulating chemical reactions PHREEQC with FEFLOW. In addition to the observed concentrations, values of $\delta^{13}C$ and $\delta^{37}C$ of 1,1,1-TCA were used for the reactive transport calibration.

After calibration, this model enhances the evaluation of 1,1,1-TCA natural attenuation based on site conditions and hydrochemical analyses. It provides also a more accurate assessment of 1,1,1-TCA degradation reactions improving the conceptual site model of natural attenuation.

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