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Self-organizing maps for groundwater quality assessment of a Belgian chalk aquifer in the presence of 1,1,1-Trichloroethane abiotic degradation

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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). The first results showed that the latter undergoes abiotic degradation by hydrolysis and dehydrohalogenation in the saturated zone. The released acids (hydrochloric and acetic acid) from these reactions influence calcite buffer action in the aquifer and change locally the water hydrochemistry.
In addition, the leaching of soluble inorganic compounds from a backfill layer has also influenced the groundwater composition in the same area. Calcium sulfate has migrated to the saturated zone with recharge water.

To confirm the first findings and elucidate the effect of each pollution source on the groundwater quality, 3 datasets from 3 annual sampling campaigns were used for Kohonen's Self-Organizing Map (SOM) analysis. The groundwater chemistry dataset used comprised: pH, electrical conductivity, Ca^{2+}, Cl^{-}, SO_4^{2-}, HCO_3^{-}, (Ca^{2+}-HCO_3^{-}), TCE, 1,1,1-TCA, 1,1-DCE and the molar ratio 1,1-DCE/(1,1,1-TCA + 1,1-DCE).

For each dataset, 3 clusters were identified within the groundwater plume. The first cluster is characterized by a chemical composition that reflects the presence of 1,1,1-TCA degradation reaction products, an increased calcite dissolution, and migration of Ca^{2+} and SO_4^{2-} from backfill soil to the groundwater. The second cluster is characterized mainly by the effect of Ca^{2+} and SO_4^{2-} migration to groundwater. The third cluster reflects the less contaminated groundwater with a composition approaching the groundwater background composition (before pollution) in the studied aquifer. The clusters spatial distribution and their chemical specifications were quite similar between the 3 datasets.

In this study, the application of SOM's is a useful tool to improve the understanding of groundwater quality changes in a contaminated site. Based on this multivariate statistical method, detection of zones influenced by two different groundwater pollution sources was possible within the studied plume.
The combination of SOM's results with the results from: backfill soil characterization, sulfate isotopic signature in groundwater, compared to the one in backfill eluates, has led to a better understanding of the ongoing mechanisms influencing hydrochemistry in this study site.

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