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Interpretation of groundwater quality patterns through groundwater modelling and Self-Organizing Map analysis

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Identification of processes affecting groundwater chemistry in unconfined aquifers requires a thorough understanding of groundwater flow and transport. In this paper travel time and spatial attributes of the infiltration area, like soil texture, land use and unsaturated zone thickness are calculated through regional groundwater modelling and used in the interpretation of groundwater quality patterns observed in an unconfined aquifer in Central Belgium.

Self Organizing Maps (SOM), a neural network technique for multi-dimensional data visualisation, is used to identify groups and relationships between solute concentrations. Groundwater modelling and particle tracking within the Generalized Likelihood Uncertainty Estimation (GLUE) framework accounts for uncertainty in hydraulic conductivity and recharge and allows the calculation of a source zone and travel time distribution for each groundwater sample. Differences in solute concentrations between the groups identified in the SOM-analysis are explained based on the average travel time and the soil texture, land use and unsaturated zone thickness in the infiltration area.

Likelihood weighted travel time and spatial attributes of the source zones for each sampling location, such as soil texture, land use and unsaturated zone thickness, show that low to medium solute concentrations are linked to grassland and longer travel times, while high solute concentrations are associated with short travel times and arable land. Oxygen-depleted samples could be subdivided in a group with low overall solute concentrations, associated with long travel times and a group with elevated solute concentrations in alluvial settings with short travel times.

The combination of multivariate data analysis and groundwater modeling not only provides a firm basis to develop a conceptual geochemical understanding of processes active in an aquifer, it has the potential to guide and evaluate existing monitoring schemes.