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## Impact of the accuracy of the conceptual geological model on predicting hot spots of redox-zones at the surface water – groundwater interface

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Managed aquifer recharge through riverbank filtration is an important method to produce drinking water in densely populated regions. Due to the discharge of wastewater into streams, this type of drinking water production can be affected by organic contaminants originating from surface water inflow. Transport and degradation of anthropogenic contaminants depend on several factors, such as pH, temperature, oxygen content, and redox conditions. One of the key factors that drive the degradation of organic contaminants like x-ray contrast media is the prevailing redox system as many pharmaceuticals and pesticides are transformed under aerobic conditions but are more persistent under anaerobic conditions.

We conducted a 1-year monitoring campaign at an active riverbank filtration plant at the Rhine river in Düsseldorf, Germany. Samples were taken every two weeks from the Rhine, a production well, and five observation wells with three different depths along a transect perpendicular to the river and parallel to the main flow direction. Samples were analyzed for main cations and anions, redox-species, and microbiological parameters. Water samples were also screened for 100 organic contaminants, pharmaceuticals, and pesticides.

A 2D reactive transport model was set-up using PFLOTRAN to simulate the redox zonation during a hydrological year. It includes aerobic respiration and denitrification with dissolved organic carbon using Monod kinetics and also accounts for temperature-dependency. Our results show that hot spots for biogeochemical processes develop close to the river, and thus most of the inflowing oxygen is already consumed within the first few decimeters. We also found a substantial seasonal variability of reaction rates due to seasonal temperature variations leading to oxygen depletion and limited denitrification in the warmest period (late summer/early fall).

Reactive transport is affected by the hydrogeological properties of the aquifer, which are influenced by its geological development. Thus, model results will depend on the reliability and accuracy of the employed conceptual geological model. Based on structural information obtained from grain size sieve analysis, and geophysical investigations such as geoelectric and natural gamma-ray measurements, we created a set of plausible conceptual models with increasing

complexity. These models range from a simple homogeneous aquifer, to a multi-layer aquifer system or a cross-bedded aquifer structure. The conceptual models include different representations of the colmation layer at the interface between river and aquifer.

Numerical analysis of the different conceptual models indicates that a homogeneous aquifer can represent a single flow path over a hydrological year. However, only more complex aquifer structures were able to reproduce the spatial and seasonal temporal variability of temperature and redox species observations ( $O_2$ ,  $NO_3^-$ ). Additionally, proper integration of the colmation layer is the key factor to simulate heat transport as well as the spatial distribution of redox-species and thus redox-zonation during the entire hydrological year, including droughts and flooding periods. Therefore, an accurate and detailed integration of the geological system into the reactive transport model, especially characteristics (e.g., size, type of material) of the colmation layer, are of highest relevance for enhanced predictions of redox zones in highly transient hydrogeological systems and at hydrodynamic interfaces.