Modelling the redox-dependent fate of a pharmaceutically active compound during managed aquifer recharge

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ABSTRACT

A reactive multi-component transport modelling study was carried out to investigate the interaction of flow and biogeochemical processes in an artificially recharged aquifer in Berlin, Germany. The modelling study elucidated and quantified the processes controlling redox zoning and the corresponding fate of the pharmaceutically active compound phenazone, an analgesic compound that was detected at several occasions in Berlins surface water and groundwater. The biogeochemical processes included in the conceptual and numerical model were (i) microbially mediated redox reactions driven by biodegradation of sediment bound organic carbon, (ii) a redox-dependent biodegradation behaviour of phenazone and (iii) several mineral reactions that affected the groundwater chemistry. The model accounted for seasonal temperature changes of the infiltration water and its influence on biodegradation reactions (higher degradation rates at higher temperatures and vice versa). The conceptual model was implemented into the reactive transport model PHT3D. The final calibrated model simulation closely reproduced the hydrogeochemical data that were recorded at 6 monitoring wells over a 2 year period. The simulation results and sensitivity analysis clearly show that the seasonal temperature variation of the infiltration water is the key factor for the observed spatial and temporal redox dynamics in the aquifer, rather than transient groundwater flow due to highly varying recharge rates. It could also be shown that the fate of phenazone solely depends on the distribution of dissolved oxygen concentration within the aquifer. Thus the degradation behaviour of phanazone is indirectly controlled by the temperature of the infiltration water. In winter, when dissolved oxygen is present within the entire investiged aquifer section phenazone becomes depleted before reaching the first monitoring well downstream of the pond. In contrast, phenazone breaks through all of the monitoring wells during summer once redox conditions have turned anoxic. The proposed modelling concept may also be applied for simulating the fate of other redox-dependend trace organic compounds in comparable hydrogeochemical systems.