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Development of a transfer function based method assessing long-term trends of solute influxes into the groundwater as a tool for quality management

Christine Kübeck, Carsten Hansen, Wolfgang van Berk, and Andreas Zervas

Institute of Groundwater Ecology, Helmholtz Zentrum Muenchen,Germany (christine.kuebeck@helmholtz-muenchen.de/+49 89 3187-3361)

In agriculturally dominated regions groundwater resources are exposed to an elevated influx of solutes from fertilizer application. Triggered by this influx subsequent hydrogeochemical processes within the aquifer often lead to the dissolution of substances relevant in water management. Therefore, the solute influx represents an important factor in groundwater quality control. However, time series needed for determination of data like the composition, amount and application intervals of agricultural additives, crop rotation (land use), climate data or hydrogechemical processes within the unsaturated zone are generally not available, or require the use of complex modeling tools for the simulation.

In order to identify effects land use practices pose on groundwater resources a conceptual model is developed assessing the influx into the groundwater in parameters like the pH and concentrations of solutes (Na+, K+, Ca+2, Mg+2, NO3-, Cl- and SO4-2). The model approach abstracts the solute influx as a function of the nitrogen surplus derived from temporal and spatial discrete mass balance calculations. Based on transfer functions, hydrogeochemical and biological processes are represented controlling the immobilization and mobilisation of substances in the unsaturated zone. The distribution of gaseous, solid and aqueous species is determined by means of thermodynamic equilibrium calculations.

Embedded into a reactive transport model, the conceptual approach enables to analyse complex interactions between the time and site specific solute influx, geohydraulic flow pattern and the geochemical-mineralogical composition of the aquifer. The reactive transport model copes with few input data derived from routinely conducted measurements of the groundwater. Thus, applied on catchment areas it provides a platform to gain insights into the prevailing hydrogeochemical processes and enables to evaluate effects of different land uses on water management. Based on this, agricultural measurements which improve or maintain quality standards of groundwater resources can be planned systematic and cost effectively.

The consistency and plausibility of the transfer function based approach is tested using the example of the agricultural dominated catchment area Forstwald (Krefeld, Germany). The production rate is about 3.6 Mio m^3 water per year. The Quaternary aquifer consists of up to 32 m thick fluvial sands and gravels (Pleistocene) of an average permeability between 0.0005 and 0.0006 m/s. The aquifer is divided into a largely oxidized upper part which contains small amounts of solid bound organic carbon (OC) and an OC-rich and pyrite-bearing lower part. Although groundwater analyses of observation wells indicate effects of variations in land use, soil composition, sorption and denitrification rates within the unsaturated zone, these processes show a low impact on raw water composition. The model reveals a strong relation between nitrate influx and iron concentration in the raw water. An increase in nitrate influx results in a partially breakthrough of nitrate to the well. The amount of ironhydroxides precipitated within the well is coupled to iron and nitrate concentrations of admixing groundwater. Thus, a reduction of fertilizers applied in the direct vicinity of the production wells can cause an increase in iron concentration at a decreasing nitrate concentration. Decreasing nitrate influxes below areas in the south of the catchment, on the other hand, may result in a time delayed elevation of nitrate concentration in raw water. Both scenarios imply a decrease in ironhydroxide precipitation. The calcium and TIC concentrations remain stable as long as carbonate phases are available within the aquifer.