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Increasing hydrological model realism and catchment knowledge with instream nitrate data

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Hydrological modelling aims to reproduce observed water fluxes, like discharge, with numerical equations. However, fitting models to observed discharge time series often results in limited new hydrological process understanding and equifinality. Recently, hydrologists address innovative ideas, e.g. by including water balance components and hydrological indices, to gain more realistic model simulations.

In this study, we increase the hydrological model realism by including daily instream nitrate concentration in a multi-objective model calibration approach. Commonly, data such as nitrate are simply seen as water quality parameters. However, biogeochemical processes that describe the turnover and transport of nitrate are tightly connected to conditions and transport processes in the unsaturated as well as saturated zones. There, matching observed and simulated nitrate concentrations requires a sound representation of the hydrological processes in the landscape. We tested our approach using six years of data of the 3.74 km^2 large Vollnkirchener Bach, which is part of the Schwingbach Critical Zone Observatory in Hesse, Germany. Nitrate concentrations are measured in-situ with a UV-hyperspectral sensor every 10 minutes and discharge every 5 minutes with an RBC-flume. Respective nitrate loads are simulated in daily resolution by coupling the regional ecosystem model LandscapeDNDC to a groundwater transport model build with CMF. Site-specific nitrate loads and percolation are simulated with LandscapeDNDC and transported to the catchment outlet with CMF. We calibrated the n=40 (n=30 for LandscapeDNDC and n=10 for CMF) model parameters following a multi-objective Bayesian approach and obtained a fair fit of the hydrograph with a NSE of 0.65 and a good fit of instream nitrate concentration data with RMSE of 0.7 mg $N\text{-}NO_3\ l^{-1}$. We found the additional consideration of the nitrate concentration highly influential on the derived posterior parameter boundaries of the hydrological model. If we focus on discharge only, we were not able to constrain the saturated conductivity parameters of the hydrological model. However, when including the nitrate data into the model calibration, we were able to identify a slow water transport under arable land use (ksat between 2-5 m day^{-1}) and a fast response under forest land use (ksat between 500-800 m day^{-1}), which corresponds with field measurements. By plotting simulated discharge and nitrate data uncertainty with their underlying spatial allocation, we are further able to assign different events to different catchment contribution areas.

This linkage of classical hydrological modelling with water quality information through process oriented biogeochemical water quality modelling helped us to reduce equifinality in our hydrological model and increase the realism of the underlying parameterization of the hydro-biogeochemical processes. We see this approach with a high potential for the hydrological community, as large-scale water quality data becomes more and more available.