

## **Grid-based water quality simulation at catchment scale: Nitrogen model development and evaluation**

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Stream water quality has been changed significantly during last few decades due to changes in human impacts. Accurate and flexible water quality models, which can properly reflect the heterogeneity and long term temporal dynamic of catchment functioning, are still needed. To this end, a new grid-based catchment water quality model was developed based on the mesoscale Hydrological Model (mHM) and the HYdrological Prediction of Environment (HYPE) model. The model structure and parameterization scheme were flexibly designed depending on the spatial heterogeneity of study sites and their specific requirements. Based on that, more detailed spatial information can be provided. Moreover, three main improvements on Nitrate sub-model were implemented: i) nitrate transport processes were conducted in physically connected river networks, allowing time-series point-source inputs added in the exact location of sewage treatment plants; ii) additional retention storage of deep groundwater was included for long term nitrate-N simulation; iii) special design for better taking into account crop rotation was implemented. Those new features can extend the model capability and facilitate the understanding of catchment mechanisms and analysis of future scenarios and measures.

The newly developed model was fully verified in the Selke catchment (456 km<sup>2</sup>), central Germany. Long term discharge and water quality data have been collected at three nested gauging stations (1997-2015). The station Meisdorf, above where 72% of area is occupied by forest, represents the discharge and nutrient exports from forest area. Agricultural land dominates the lower part of the catchment (almost 96% of in-between area of the Meisdorf and the outlet station Hausneindorf) with considerable urban areas. Due to the relatively large number of model parameters, sensitivity analysis was firstly conducted. Subsequently, sensitive parameters were calibrated using stepwise and multi-variable approaches, respectively. Results showed that the latter approach outperforms the former one, reflecting that water quality data contains important hydrological information (i.e. runoff partitioning), which could not be reflected in stream water discharge and should be used to constrain hydrological modeling. The simulation fitted observations nicely in both discharge (NSEs at three stations were 0.68, 0.81 and 0.85 respectively) and nitrate-N concentration (NSEs were 0.38, 0.57 and 0.70 respectively). Furthermore, the calibrated model has also been used to test the explanation of long-term dynamic of nitrate-N observations at station Hausneindorf, whose seasonal pattern has changed dramatically. Three possible contributions can be summarized as: input from the upper forest areas (station Meisdorf), export from the lower agricultural lands and point-source pollution in considerable urban areas. Long term simulation at the outlet showed that the model could nicely reproduce changes of flow components and the associated changes in nitrogen concentration patterns.