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A high-resolution conceptual model for diffuse organic micropollutant loads in streams

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The ecological state of surface waters has become the dominant aspect in water quality assessments. Toxicity is a key determinant of the ecological state, but organic micropollutants (OMP) are seldom monitored with the same spatial and temporal frequency as for example nutrients, mainly due the demanding analytical methods and costs. However, diffuse transport pathways are at least equally complex for OMPs as for nutrients and there are still significant knowledge gaps. Moreover, concentrations of the different compounds would need to be known with fairly high temporal resolution because acute toxicity can be as important as the chronic one. Fully detailed mechanistic models of diffuse OMP loads require an immense set of site-specific knowledge and are rarely applicable for catchments lacking an exceptional monitoring coverage. Simple empirical methods are less demanding but usually work with more temporal aggregation and that's why they have limited possibilities to support the estimation of the ecological state.

This study presents a simple conceptual model that aims to simulate the concentrations of selected organic micropollutants with daily resolution at 11 locations in the stream network of a small catchment (46 km^2). The prerequisite is a known hydrological and meteorological background (daily discharge, precipitation and air temperature time series), a land use map and some historic measurements of the desired compounds.

The model is conceptual in the sense that all important diffuse transport pathways are simulated separately, but each with a simple empirical process rate. Consequently, some site-specific observations are required to calibrate the model, but afterwards the model can be used for forecasting and scenario analysis as the calibrated process rates typically describe invariant properties of the catchment.

We simulated 6 different OMPs from the categories of agricultural and urban pesticides and urban biocides. The application of agricultural pesticides was also simulated with the model using a heat-sum approach. Calibration was carried out with weekly aggregated samples covering the growing season in 2 years. The model could reproduce the observed OMP concentrations with varying success. Compounds that are less persistent in the environment and thus have a dominant temporal dynamics (pesticides with a short half-life) could be simulated in general better than the persistent ones. For the latter group the relatively stable available stock meant that there were no clear seasonal dynamics, which revealed that transport processes are quite uncertain even when daily rainfall is used as the main driver. Nevertheless the daily concentration distribution could still be simulated with higher accuracy than the individual peaks. Thus we can model the concentration-duration relationship for daily resolution in an acceptable way for each compound.