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Modeling concentration patterns of agricultural and urban micropollutants in surface waters in catchment of mixed land use

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Organic micropollutants detected in surface waters can originate from agricultural and urban sources. Depending on the use of the compounds, the temporal loss patterns vary substantially. Therefore models that simulate water quality in watersheds of mixed land use have to account for all relevant sources. We present here simulation results of a transport model that describes the dynamic of several biocidal compounds as well as the behaviour of human pharmaceuticals. The model consists of the sub-model Rexpo simulating the transfer of the compounds from the point of application to the stream in semi-lumped manner. The river sub-model, which is programmed in the Aquasim software, describes the fate of the compounds in the stream. Both sub-models are process-based.
The Rexpo sub-model was calibrated at the scale of a small catchment of 25 km2, which is inhabited by about 12'000 people. Based on the resulting model parameters the loss dynamics of two herbicides (atrazine, isoproturon) and a compound of mixed urban and agricultural use (diuron) were predicted for two nested catchment of 212 and 1696 km2, respectively. The model output was compared to observed time-series of concentrations and loads obtained for the entire year 2009. Additionally, the fate of two pharmaceuticals with constant input (carbamazepine, diclofenac) was simulated for improving the understanding of possible degradation processes.
The simulated loads and concentrations of the biocidal compounds differed by a factor of 2 to 3 from the observations. In general, the seasonal patterns were well captured by the model. However, a detailed analysis of the seasonality revealed substantial input uncertainty for the application of the compounds. The model results also demonstrated that for the dynamics of rain-driven losses of biocidal compounds the semi-lumped approach of the Rexpo sub-model was sufficient. Only for simulating the photolytic degradation of diclofenac in the stream the detailed representation of the routing in the stream was essential.
Overall, the study demonstrated that the simulation of micropollutants at the watershed scale can be strongly hampered by input uncertainty regarding the use of the chemicals. Under such conditions the level of process-representation in the Rexpo sub-models is superfluous. For practical applications, one should address the question how to simply the approach while still maintaining the essential parts.