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Fate of micropollutants at catchment scale and prediction of river concentrations. Which model to choose? A case study for perfluorinated compounds in Austria

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With an exponentially growing number of micropollutants dispersed in the environment and an increasing financial effort associated with the detection of very low concentrations in water bodies, models at catchment scale have become an essential tool to identify potential hotspots, to prioritize monitoring campaigns and to support river basin management plans. The choice of the model approach generally brings with it compromises between complexity and accuracy and depends on the specific goals and needs. In this work we compare and critically discuss the performance and the suitability of two different modelling approaches applied at the mesoscale (catchments area between 9 km^2 and 300 km^2). We present the results for two perfluorinated compounds, namely Perfluorooctanoic acid (PFOA) and Perfluorooctanesulfonic acid (PFOS). Both are well-known hazardous pollutants, but not much is known about the spatial distribution of the contamination in river basins.

The first model (MoRE, Modeling of Regionalized Emissions) is a relatively data intensive, semi-empiric tool conceived for regionalized pathway analysis. We applied it in all Austrian river catchments to estimate yearly loads and annual mean concentrations. The parametrization relied on a targeted monitoring and on composite samples across several environmental compartments (Zoboli et. al., 2019). We validated the model at 12 quality measurement stations with yearly loads and annual mean concentrations. The second tool is a fate process-based model train developed within the EU SOLUTIONS project for the Danube River Basin (Lindim et al., 2016), which we validated at the same water quality stations. The model train estimates daily concentrations based on emissions and substance properties. It requires only few regional data, mainly regarding hydrology, and thus the parametrization is much easier.

The MoRE model showed very good agreement for the loads for PFOA (NSE 0.81, mNSE 0.68) and PFOS (NSE 0.89, mNSE 0.76) and partially good agreement regarding the annual mean concentrations: PFOA (R^2 0.41, NSE 0.22, mNSE 0.11) and PFOS (R^2 0.8, NSE 0.73, mNSE 0.53). The

SOLUTIONS model train showed a systematic overestimation of annual mean concentrations for most of the stations for PFOA (R^2 0.19, NSE -5.1, mNSE -0.78) and PFOS (R^2 0.61, NSE -9.5, mNSE -1.4). As our observation data consist of long-term composite samples, we were not able to compare the daily concentrations given by the model with the samples. Thus, we could not investigate the temporal pattern of the model deviation.

Despite some limitations, the comparison indicates that the higher parametrization effort required by the MoRE model yields more accurate results. Where parametrization data is available, MoRE shall be preferred, since it also provides information about the contribution of different emission pathways (e.g. groundwater and interflow, wastewater treatment plants, industry) to the total emissions. SOLUTIONS brings clear advantages when parametrization data is scarce or for very large river basins. However, it would benefit from a further refinement based on the more detailed system understanding provided by MoRE. A future line of research would thus be their parallel application in combination with a targeted monitoring able to cover both spatial and temporal variability.