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Suitability of regulatory data to predict micropollutant degradation in rivers

Mark Honti (1), Fabian Bischoff (2), Andreas Moser (2), Christian Stamm (2), and Kathrin Fenner (2)

(1) MTA-BME Water Research Group, Hungarian Academy of Sciences, Budapest, Hungary (mark.honti@gmail.com), (2) EAWAG Department of Environmental Chemistry, Dübendorf, Switzerland

For many chemicals a certain loss to surface water bodies over their life-cycle is unavoidable. These include pesticides, human pharmaceuticals, biocides, industrial chemicals, and veterinary medicines. Since most of them possess an intentional biological activity, they bear the potential to harm non-target organisms in the environment. The actual exposure to a chemical in the environment after emission is determined by its persistence, i.e. by the rate at which it is removed by biological and chemical degradation processes. For surface water systems, major transformation processes include chemical hydrolysis, direct and indirect photo-transformation and microbial bio-transformation.

Laboratory-based test systems play an important role in evaluating chemical transformation for regulatory purposes due to their replicability, their lower costs compared to field tests, and the better representation of environmental systems compared to lower tier biodegradability and hydrolysis tests.

The OECD 308 and 309 test systems are relevant for evaluation of microbial biotransformation of chemicals in surface waters. Degradation half-lives derived from these experiments are typically used in exposure modeling and persistence assessment. These “simulation” tests have been severely criticized for yielding results strongly specific to the experimental systems and for therefore being irrelevant for most environmental conditions.

Our objective was to check the relation between degradation half-lives measured in regulatory tests and half-lives observed in actual surface water bodies. We used the Rhine river catchment and the results of a field campaign carried out in 2011 (Ruff et al. 2015, Water Research). 7 pharmaceuticals were selected, including a conservative benchmark substance. Laboratory degradation half-lives were extracted from OECD 308 data. A GIS model was set up to simulate the accumulation of chemicals from the wastewater treatment plants of the catchment and the behavior of the chemicals in the river Rhine.

For substances with OECD 308 data, predictions using compartment-specific degradation half-lives were found to be in accordance with measured concentrations, but not much different from simulations assuming no degradation. This suggests that the usually fairly long water half-lives dominated the compounds’ behavior in the river Rhine. Besides this, it highlighted that the shorter total system half-lives derived from OECD 308 are indeed irrelevant for assessing persistence in medium to large river systems. For two substances, it was not possible to tune modelled concentration patterns to be in agreement with observed data, even when assuming different extents of degradation. This underlined the influence of input uncertainty (e.g. consumption in different countries and regions).

Finally, the model was used to investigate what kind of water half-lives would result in an observable degradation along the Rhine. Substances with half-lives shorter than 9 days would show spatial concentration patterns that are clearly different from those of a conservative benchmark chemical, given the typical measurement, model and input uncertainty. Besides learning the inadequacy of certain indicators from laboratory simulation studies for assessment of environmental persistence, our results suggest that emissions of many organic micropollutants showing observable degradation in the laboratory are transferred almost without loss to the sea, even from such a large river basin as the Rhine.