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Re-evaluation of the sorption behaviour of Bromide and Sulfamethazine under field conditions using leaching data and modelling methods

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The simulation of reactive transport in the aquatic environment is hampered by the ambiguity of environmental fate process conceptualizations for a specific substance in the literature. Concepts are usually identified by experimental studies and inverse modelling under controlled lab conditions in order to reduce environmental uncertainties such as uncertain boundary conditions and input data. However, since environmental conditions affect substance behaviour, a re-evaluation might be necessary under environmental conditions which might, in turn, be affected by uncertainties. Using a combination of experimental data and simulations of the leaching behaviour of the veterinary antibiotic Sulfamethazine (SMZ; synonym: sulfadimidine) and the hydrological tracer Bromide (Br) in a field lysimeter, we re-evaluated the sorption concepts of both substances under uncertain field conditions.

Sampling data of a field lysimeter experiment in which both substances were applied twice a year with manure and sampled at the bottom of two lysimeters during three subsequent years was used for model set-up and evaluation. The total amount of leached SMZ and Br were 22 μg and 129 mg, respectively. A reactive transport model was parameterized to the conditions of the two lysimeters filled with monoliths (depth 2 m, area 1 m^2) of a sandy soil showing a low pH value under which Bromide is sorptive. We used different sorption concepts such as constant and organic-carbon dependent sorption coefficients and instantaneous and kinetic sorption equilibrium. Combining the sorption concepts resulted in four scenarios per substance with different equations for sorption equilibrium and sorption kinetics. The GLUE (Generalized Likelihood Uncertainty Estimation) method was applied to each scenario using parameter ranges found in experimental and modelling studies. The parameter spaces for each scenario were sampled using a Latin Hypercube method which was refined around local model efficiency maxima.

Results of the cumulative SMZ leaching simulations suggest a best conceptualization combination of instantaneous sorption to organic carbon which is consistent with the literature. The best Nash-Sutcliffe efficiency (Neff) was 0.96 and the 5th and 95th percentile of the uncertainty estimation were 18 and 27 μg. In contrast, both scenarios of kinetic Br sorption had similar results (Neff =0.99, uncertainty bounds 110-176 mg and 112-176 mg) but were clearly better than instantaneous sorption scenarios. Therefore, only the concept of sorption kinetics could be identified for Br modelling whereas both tested sorption equilibrium coefficient concepts performed equally well. The reasons for this specific case of equifinality may be uncertainties of model input data under field conditions or an insensitivity of the sorption equilibrium method due to relatively low adsorption of Br.

Our results show that it may be possible to identify or at least falsify specific sorption concepts under uncertain field conditions using a long-term leaching experiment and modelling methods. Cases of environmental fate concept equifinality arouse the possibility of future model structure uncertainty analysis using an ensemble of models with different environmental fate concepts.