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Simulation of the long-term behaviour of Sulfamethazine in two different soils using the MACRO model

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The sulfonamide Sulfamethazine (SMZ) is one of the most commonly used antibiotic agents in the field of veterinary medicine. SMZ has been shown to be released into the environment via the application of contaminated farm fertilizer. The fate of SMZ in soils and the consequences of a regular entry are not yet clearly investigated due to the complexity of interactions in soils. Still, it has been shown, that leaching can occur over several years. At this point simulation programs can contribute to a better understanding of the environmental behaviour. The pesticide leaching model MACRO 5.2 is a commonly used program in the pesticide registration procedure of the EU. The suitability of MACRO for the simulation of the long-term behaviour of SMZ is tested in this study. A lysimeter study carried out on two different sites in Lower Saxony (Germany) over a period of seven years provides the sampling data basis.
For the calibration process the Monte Carlo approach is used for generating different parameter combinations. After calibrating soil properties considering available bromide-leaching data, the parameter values resulting in the highest KGE are taken as basis for the SMZ simulation. This step is necessary due to uncertainties associated with the SMZ data. The main focus of this study lies in reproducing the long-term behaviour of SMZ by including a kinetic sorption, whereby no degradation takes place on kinetic sites, and an irreversible sorption. MACRO is not capable of simulating the latter. Therefore, a first order degradation rate on equilibrium sorption sites has to be included. In a second step the ranked pearson partial correlation coefficient (RPCC) is calculated for every time step to identify the time-dependent sensitivity of parameters included in the calibration process. Based on the simulations, the time dependent distribution of potentially mobile SMZ in each soil layer is identified and compared to the maximum allowed predicted environmental concentration in soils for veterinary medicinal products.
The Monte Carlo simulations indicate, that it is possible to reproduce the behaviour of SMZ with the MACRO model under the condition of including three sorption sites: a fast equilibrium sorption, a slower kinetic sorption and an irreversible sorption.