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Simulating PFOS and PFOA leaching under field conditions using the MACRO model

Matthias Gassmann (1), Eva Weidemann (1), Kai Sonntag (1), and Thorsten Stahl (2)

(1) University of Kassel, Institute for Water, Waste, Environment, Water Quality Management - Modelling and Simulation, Kassel, Germany (gassmann@uni-kassel.de), (2) Hessian State Laboratory, Kassel, Germany

Due to their surfactant, water and oil repellent, catalytic and stable nature, perfluoroalkyl substances (PFAS) are used in industrial production and manufacturing for various purposes. In recent years, widespread contamination of soil, groundwater, drinking water, feed and food were identified at various places (so called “hot spots”) in Germany, caused by contaminated compost and sewage sludge used as fertilizer. Besides their preferential adsorption to organic carbon, the environmental fate of PFAS is generally different to other organic compounds in the environment such as pesticides: PFAS are mostly not biodegradable in soil, their removal from the soil column is rather an effect of partially irreversible adsorption, a process which is not yet fully understood. While there is a large variety of leaching models developed and tested for pesticides, no attempt has been made to simulate the long-term fate of PFAS in soils so far.

In this study, we applied the MACRO model, which was developed for the estimation of pesticide transfer in soils, for leaching simulations of perfluorooctane sulfonate (PFOS) and perfluorooctanoic acid (PFOA), which are generally treated as lead substances among PFAS. The model was set up by using soil and crop rotation data of a long-term field lysimeter study investigating the behaviour of PFOS and PFOA over a period of eight years. Since irreversible adsorption is not explicitly considered in MACRO, we used degradation in the adsorbed phase in order to mimic this process. Using this setup, the MACRO model was able to reproduce water and substance leaching within parameter ranges taken from the literature. In addition to the information provided by sampling data, the model results indicate that more than 95 % of both substances is irreversibly adsorbed to soils after the 8-years period. About 4 % of PFOS is still in the mobile adsorption pool at the end of the simulation period, showing that the soil passage of this substance is not yet finished. In contrast, PFOA passage is largely finished (less than 0.01% in the mobile pool). The dynamics of plant uptake could only partially be reproduced with the highest uptake in the first season after substance application. Uptake in later years could not be modelled well which might have been an effect of the constant transpiration stream coefficient for each plant species in the command line version of the MACRO model or the relatively simple root growth model. Concluding, the MACRO model can be used for the simulation of PFOS and PFOA leaching in soils by using a work-around model setup with degradation in the adsorbed phase mimicking irreversible adsorption. Since PFAS are not the only chemicals in the environment affected by irreversible adsorption, this process should be given more attention in experimental and simulation studies.