Geophysical Research Abstracts
Vol. 20, EGU2018-648, 2018
EGU General Assembly 2018

Prediction of two surfactants to the soil solid phase based on Mid-Infrared Spectroscopy and Partial Least Square Analysis.

Melanie Wisgott (1), Jannis Heil (), Bernd Marschner (2), and Britta Stumpe ()

(1) University of Wuppertal, Geography, Human and Environmental Research, Germany (wisgott@uni-wuppertal.de), (2) University of Bochum, Geography, Soil Science/Soil Ecology, Germany (bernd.marschner@rub.de)

Persistent organic pollutants (POPs) are known to have adverse effects on human health and the environment. Thus, an effective risk assessment with concern on POP adsorption potential in the soil compartment is of high interest.
The objective of our study was to develop a reliable, rapid and low-cost method which is able to predict the adsorption of two model POPs, 4-n-nonylphenol (NP) and perfluorooctanoic acid (PFOA), in soil samples based on spectral information (MIR) and partial least-square analyses (PLSR).
For the model development 96 top- as well as subsoils were used. To characterize the composition of the samples, they were analyzed for particle size distribution, manganese and iron oxide concentration, organic carbon content (SOC), pH and the soil surface area. The KD-values for NP and PFOA were calculated in batch experiments. FT-IR spectra of all samples were measured in the mid-infrared region after soil sieving (< 2mm) and after an additional grinding procedure (< 0.01 mm).
NP and PFOA are selected as model pollutants since they are highly resistant against microbial degradation. As consequence their environmental fate will be mainly controlled by adsorption and desorption processes in soils. MIR spectroscopy was used to predict the sorption of NP and PFOA, because it reflects the total soil composition. Generally, the adsorption of NP and PFOA was linear in all soil samples. However, significant differences between the KD values of PFOA (log(KD)= 0.1-27.6 ml g-1) and NP (log(KD)= 60-4,840 ml g-1) have been observed. The multiple regression analysis revealed that the PFOA adsorption was mainly controlled by the soil organic carbon content as well as by the iron oxide content. The NP adsorption only depended on the SOC content. Since different adsorption mechanisms of NP and PFOA have been observed we decide to develop different prediction models for both pollutants.
The partial least square regression combined with the Infrared data was able to predict the sorption behavior of PFOA better (R^2 = 0.86) than for NP (R^2 = 0.79). Since the sorption was mainly influenced by the SOC content, it was interesting to know if the sorption behavior changes with lower carbon contents. The results showed that the accuracy of the prediction decreases, when only samples with SOC contents lower than 1.5 % are considered. Nevertheless, these results are indicating, that models based on MIR spectroscopy are able to predict the sorption behavior of Nonylphenol und perfluorooctanoic acid.