Characterization of sorption of organic compounds by polyethylene using poly-parameter linear free-energy relationships

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Plastic debris in the aquatic environment has become a major concern. Potential input pathways of these materials may be either in the form of direct littering or through industrial waste as filling materials or abrasives from cosmetics. Once released into the environment, plastics can degrade through various processes (e.g., UV, mechanical, or biological) into smaller particles of sizes below 5 mm, which are called microplastics (MP). Recent studies have shown that MP can be ingested by marine organisms, such as mussels or water fleas, and may thereby consequently accumulate in the food chain. In conjunction with the ingestion by organisms, it is also discussed whether the phase transfer between water and plastic or enhanced bioaccumulation of persistent organic pollutants may occur as a result of the high sorption affinity and capacity of many plastics for lipophilic compounds.[1] The interaction between plastics and neutral organic substances in water is important in many areas, for example leaching of plastic packaging or diffusion into freshwater pipes. Plastics in the environment can sorb persistent organic pollutants and transport them into non-polluted areas, slowly releasing them through desorption. To date, the research focus has clearly been on the occurrence and characterization of MP in the environment, while there is little information available describing sorption by these materials. Thus, a better understanding of the sorption properties of plastics is necessary for a risk assessment to aquatic ecosystems.

Methods for the prediction of sorption based on one-parameter linear free energy relationships using for example the octanol-water partitioning constant, log $K_{O/W}$, are commonly used for a wide range of sorbent-sorbate systems. However, these approaches often lack the accurate and precise prediction of sorption and are transferable from one compound class to another.

Thus, in this work sorption by polyethylene (PE) was characterized using a poly-parameter model published by Abraham et. al.[2]. This model describes sorption more accurate than commonly used one-parameter approaches due to the use of both sorbate and phase descriptors. These models can be used for an *a priori* prediction of sorption by the characterized sorbent materials. To this end, sorption batch experiments with well-chosen probe sorbates were carried out in a two-phase system (water/polyethylene) covering an aqueous concentration range of at least three orders of magnitude. Multiple regression analysis using the determined distribution coefficients and literature-tabulated sorbate descriptors was performed to obtain the phase descriptors for PE[3]. For independent validation of the derived ppLFER model, distribution coefficients of five additional compounds were predicted and compared with the experimental data.

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