**Sorption of anionic and neutral species of organic acids to carbonaceous sorbents - mechanisms and prediction**

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Many contaminants of concern are organic acids that dissociate under environmental conditions, and may thus exist as neutral and/or anionic species. The sorption of dissociated organic acids to carbonaceous sorbents e.g., soot, activated carbon, is typically lower than that of neutral species, but it is driven by complex processes that are not yet fully understood, and may dominate sorption in environmental matrices. Predictive approaches developed for neutral compounds and based on log Kow, are unlikely to be suitable for organic acids, due to the effects of dissociation on sorption. Previous studies on the sorption of organic acids to soils have demonstrated that log D, which describes the decrease in hydrophobicity of acids as a result of dissociation, is a useful alternative to log Kow [1,2].

The aim of the present study was to test the applicability of log D based approach to describe the sorption of acidic compounds to carbonaceous sorbents. Batch experiments were performed with a series of 15 materials including carbon nanotubes, activated carbon, and a variety of biochars (produced from different feedstock materials and temperature) and four acidic compounds commonly used for pesticidal and biocidal purposes (i.e., 2,4-D, MCPA, 2,4-DB, and triclosan). The wide range of properties considered allows (i) discussing the mechanisms driving the sorption of neutral and anionic species to carbonaceous sorbents, and (ii) their dependency on sorbate and sorbent properties.

Results showed that the sorption of the four acids was influenced by factors that are usually not considered for neutral compounds (e.g., ash content and pH). Dissociation affected the sorption of the four compounds, and sorption of the anions ranged over five orders of magnitude, thus substantially contributing to sorption in some cases. For prediction purposes, most of the variation in sorption (>80%) could be well described with a two-parameter regression equation including log D and specific surface area. The proposed model may serve as a base to estimate the environmental fate of organic acids in the presence of carbonaceous sorbents.

References:

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[2] Kah M, Brown CD. LogD: lipophilicity for ionisable compounds. Chemosphere 2008;72:1401–8. doi:10.1016/j.chemosphere.2008.04.074.