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Predicting sorption of organic acids to a wide range of carbonized sorbents

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Many contaminants and infochemicals are organic acids that undergo dissociation under environmental conditions. The sorption of dissociated anions to biochar and other carbonized sorbents is typically lower than that of neutral species. It is driven by complex processes that are not yet fully understood. It is known that predictive approaches developed for neutral compounds 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 Dow, which describes the decrease in hydrophobicity of acids upon dissociation, is a useful alternative to log Kow. The aim of the present study was to adapt a log Dow based approach to describe the sorption of organic acids to carbonized sorbents. Batch experiments were performed with a series of 9 sorbents (i.e. carbonized wood shavings, pig manure, and sewage sludge, carbon nanotubes and activated carbon), and four acids commonly used for pesticidal and biocidal purposes (i.e. 2,4-D, MCPA, 2,4-DB, and triclosan). Sorbents were comprehensively characterized, including by N2 and CO_2 physisorption, Fourier transform infrared spectroscopy, and elemental analysis. The wide range of sorbents considered allows (i) discussing the mechanisms driving the sorption of neutral and anionic species to biochar, 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 (i.e. pH, ionic strength). 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 to carbonized sorbents (89%) could be well described with a two-parameter regression equation including log Dow and sorbent specific surface area. The proposed model may serve as a base to estimate the environmental fate of organic acids in the presence of carbonized sorbents such as biochar, and help assess (i) the potential application of biochar for remediation purposes and (ii) the potential effect of biochar addition to soil.