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Agricultural Research Service, Saint Paul, United States



## Understanding mechanisms to predict and optimize biochar for agrochemical sorption

Kathleen Hall (1), Beatriz Gámiz (2), Lucia Cox (2), Kurt Spokas (3), and William Koskinen (1) (1) University of Minnesota, Department of Soil, Water and Climate, Saint Paul, MN USA (hall0995@umn.edu), (2) Instituto de Recursos Naturales y Agrobiología de Sevilla (IRNAS-CSIC), Sevilla, Spain, (3) United States Department of Agriculture,

The ability of biochars to bind various organic compounds has been widely studied due to the potential effects on pesticide fate in soil and interest in the adoption of biochar as a "low-cost" filter material. However, the sorptive behaviors of biochars are extremely variable and much of the reported data is limited to specific biochar-chemical interactions. The lack of knowledge regarding biochar sorption mechanisms limits our current ability to predict and optimize biochar's use. This work unveils mechanistic drivers of organic pesticide sorption on biochars through targeted alteration of biochar surface chemistry. Changes in the quantity and type of functional groups on biochars and other black carbon materials were achieved through treatments with H<sub>2</sub>O<sub>2</sub>, and CO<sub>2</sub>, and characterized using Fourier transform infrared spectroscopy and scanning electron microscope (SEM/EDX). The sorption capacities of these treated biochars were subsequently measured to evaluate the effects of different surface moieties on the binding of target herbicides cyhalofop acid ((R)-2-[4-(4-cyano-2-fluorophenoxy)phenoxy]propionic acid) and clomazone (2-[(2-chlorophenyl)methyl]-4,4-dimethyl-1,2-oxazolidin-3-one). Sorption of both herbicides on the studied biochars increased following H<sub>2</sub>O<sub>2</sub> activation; however, the influence of the H<sub>2</sub>O<sub>2</sub> activation on sorption was more pronounced for cyhalofop acid (pKa = 3.9) than clomazone, which is non-ionizable. Increased cyhalofop acid sorption on H<sub>2</sub>O<sub>2</sub> treated biochars can be attributed to the increase in oxygen containing functional groups as well as the decrease in biochar pH. In contrast, CO<sub>2</sub> activation reduced the sorption of cyhalofop acid compared to untreated biochar. FTIR data suggest the reduced sorption on CO<sub>2</sub> -treated biochar was due to the removal of surface carboxyl groups, further supporting the role of specific functionality in the sorption of ionizable herbicides. Results from this work offer insight into the mechanisms of sorption and provide the basis to simultaneously evaluate the overall effectiveness of surface activation treatments. In addition, we are currently examining the influence of specific biochar alterations via activation on nitrate sorption and uptake; forthcoming results will also be presented.