Predicting 2,4-dintroanisole (DNAN) sorption on various soil "types" using different compositional datasets

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Soil heterogeneity is a major contributor to the uncertainty in predicting the environmental fate of data-scare contaminants. Here, we focused on research designed to predict the soil environmental fate of the new munition compound, called 2,4-dintroanisole (DNAN) -a compound increasingly employed by the U.S. and international militaries in the next-generation, insensitive explosive formulations. We collected composite soils classified under the Ultisols taxonomic Order in the U.S. NRCS soil classification system, quantified their properties via physical and chemical characterizations, and developed quantitative analogies using compositional data analysis (CoDa), that allowed for partitioning the characterization data into four different compositions: Water-extracted (WE), Mehlich-III extracted, particle-size distribution, and solid-phase carbon-nitrogen-sulfur compositions. Prediction models testing the correlation of the DNAN sorption distribution coefficients (K_D) values to the centered logratio -transformed compositions were calculated using CoDa-modified multilinear regression. Results showed that DNAN sorption was only predictable with the WE composition, and four important variables related to equilibrium dissolved organic carbon, pH, and the exchange cations Ca and K. Analogies for DNAN sorption were the most discriminating at the Suborder level because of the inherent ambiguity in the Hapludults class at the Great Group level.