

Molecular dynamics simulation and experimental study of the adsorption of phthalate esters on clay surfaces

JENNIFER WILLEMSSEN, IAN BOURG

Princeton University, Princeton, NJ 08544, USA

(jarw@princeton.edu, bourg@princeton.edu)

Phthalate esters are plasticizers added to a wide range of products to increase flexibility. Their ubiquitous use, tendency to leach into water sources, and endocrine disrupting properties have made phthalates emerging organic contaminants (EOCs) of concern. Understanding the processes fundamental to the transport and persistence of EOCs in the environment is essential for developing remediation strategies. Central to this is the adsorption of EOCs by soils. The affinity of organic molecules for soils can result in substantial water-soil partitioning, and adsorption can restrict molecular transport and hinder bacterial and photo degradation.¹ Studies have indicated that the clay content of a given soil can play a substantial role in the partitioning², but the relevant mineral-organic interactions are not fully understood. In this research, we present a molecular dynamics (MD) simulation methodology to model a stack of flexible Ca-smectite sheets in contact with a bulk aqueous reservoir containing phthalate molecules of interest. From the simulation output, we can determine the extent of adsorption and gain insights into the partitioning behaviour of the phthalate molecules. In particular, we calculate the free energy of adsorption, the affinity of the organic compounds for different clay adsorption sites (interlayer, edge, external basal surface), and the impact of adsorption on clay basal spacing. Simulation results are compared to collected experimental adsorption, FTIR, and XRD data.

[1] Kleber M, *et al.* Adv Agron 130:1 (2015). [2] Pils J & Laird D, Environ. Sci. Technol 41:1928 (2007).