Behavior of water in a lipid-clay film

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Assembly of the lipid fraction of soil organic matter on mineral surfaces may stabilize lipids against microbial attack and the consequent redistribution of carbon. However, such assembly is a poorly understood phenomenon that reflects underlying lipid-lipid and lipid-substrate interactions, both of which are expected to be sensitive to hydration/dehydration cycles and have the potential for significant environmental impacts. For example, lipid-substrate interactions have been implicated in seasonal changes in soil water repellency. Therefore, it is desirable to build a molecular-scale understanding of lipid-mineral interactions. To build that understanding, we used a simple model system of two phosphoethanolamine lipids and the clay montmorillonite. We conducted atomic force microscopy and fluorescence microscopy experiments to determine the structure of the film and the distribution of lipids within it, and compared these results to the measured wettability of the film. We performed molecular dynamics simulations of phospholipid-montmorillonite interaction to determine the structure of lipid aggregates and the nature of their interaction with montmorillonite surfaces.

We characterized the wettability of the lipid-clay films by measuring the initial contact angle, a rate constant for droplet spreading via infiltration, and the fluid index of water in contact with the film. For these films, water behaves as a shear-thinning fluid during infiltration. Surpisingly, the nanoscale distribution of lipid aggregates on the film surface had little effect on wettability, while the microscale lipid distribution and film topography had the most influence. The physical state of the lipids – solid vs. liquid – alters film wettability, even if the solid and liquid lipids have similar distributions within the film. In order to explain why the state of the lipid alters parameters such as the fluid index of water, we hypothesize that the solid lipids alter the pore size in the film, therefore changing the effect of confinement on the properties of water. On the other hand, the liquid lipids are more likely to solubilize and detach from the mineral surfaces.