A molecular dynamic study of Soil Organic Matter stabilization mechanisms

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It is well known that some fractions of soil organic matter (SOM) can resist to physical and (bio)chemical degradation which can be attributed to factors ranging from molecular properties to the preference for digesting other molecular species by microorganisms. Some mechanisms, by which organic matter is protected, are often referred to as: physical stabilization through microaggregation, chemical stabilization by formation of SOM-mineral aggregates, and biochemical stabilization through the formation of recalcitrant SOM.

Protection mechanisms are responsible for the accumulation process of organic carbon, reducing the exposure of organic matter and making it less vulnerable to microbial, enzymatic or chemical attacks. In these mechanisms, water molecular bridges and metal cation bridges play a key role. Cation bridges serve as aggregation sites on humic substances, forming dense matter, in comparison to systems where bridges are missing. This effect is enhanced in systems with cations at higher oxidation states.

By using the modeler tool developed in our group (Vienna Soil–Organic–Matter Modeler, VSOMM2) (Escalona et al., 2021), we generated aggregate models of humic substances at atomistic scale reflecting the diversity in composition, size and conformations of the constituting molecules. Further, we built models of organo-clay aggregates using kaolinite and montmorillonite as typical soil minerals. This allowed a systematic study to understand the effect of the surrounding environment at microscopic scale, not fully accessible experimentally.

Molecular simulations of the adsorption process of SOM aggregates on the reactive surfaces of led to two observations: 1) the humic substances aggregates were able to interact with the reactive surfaces mainly via hydrogen bonds forming stable organic matter-clay complexes and 2) the aggregates subsequently lost rigidity and stability after metal cations removing, consequently leading to a gradual loss of humic substance molecules, evidencing the role of metal cations in the protection mechanism of soil organic matter aggregates and possibly explaining its recalcitrance (Galicia-Andrés et al., 2021).

References