Geophysical Research Abstracts
Vol. 21, EGU2019-14176-1, 2019
EGU General Assembly 2019

Modeling the formation of soil microaggregates

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The functions of soils are intimately linked to its aggregated structure that is formed during pedogenesis. At the basis of soil structural hierarchy, microaggregates are the smallest conceivable compounds built from a vast variety of mineral, organic, and biotic materials. Qualitative hypotheses and concepts on how aggregates form are quite elaborate but the consistent quantitative application within a mechanistic and physically rigorous framework is still missing. This is partly caused by the fact that such an endeavor requires the combination of synergistic concepts on the (random) movement of particles and their interactions affected by shape, size, and surface properties in aqueous suspensions. Here we present a novel quantitative approach for the formation of soil microaggregates that integrates diffusion-limited cluster-cluster aggregation with a probabilistic adhesion/detachment following the Derjaguin-Landau-Verwey-Overbeek (DLVO) theory of particle interactions. To represent universal mineral shapes found in soils, we implemented spherical, plate-like as well as rod-like particle morphologies inspired by weathered silicates, secondary clay minerals and pedogenic iron oxides. In this way, we developed a model that reproduces three-dimensional structural dynamics of aggregates emerging from hetero- as well as homo-aggregation in response to the physicochemical milieu. We then exploited the 3D morphology to assess crucial functional properties of aggregates exemplified with the water retention curve and the pore size distribution. Thus, a heuristic relation of soil suspension properties (physicochemistry, mineralogy) and the development of aggregate structure could be drawn that may help to identify mechanisms and factors controlling microaggregate dynamics.