A stochastic approach on aggregate development based on diffusion-limited aggregation

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Soil functions are instrinsically related to the composition, structure, and stability of soil aggregates. Of particular importance in the system of aggregates are microaggregates [1] smaller <250µm and their composite building units, which are associations of minerals and soil organic matter with an internal pore structure accessible for microbes and solutes. The mechanisms and rates of initial development of composite building units are poorly understood by now. We present a stochastic bottom-up approach to describe aggregate formation from basic building units in aqueous solutions, which is one presumed pathway of formation. It is based on the combination of diffusion-limited aggregation [2] with the extended DLVO theory to describe interaction energies between particles. Basic geometric body classes were used to resemble the general shape of mineral particles. The model outcomes are compared to data obtained by SEM and X-RAY µ-CT. We demonstrate that the interplay of geometric bodies if governed by this limited set of "physical rules" results in complex structured aggregates that feature similar properties as their natural counterparts. As a result, comprehensive sensitivity analyses relating local properties of building units to aggregate scale phenomena are possible. We systematically tested the influence of particle density, shape and interaction energies. First results revealed the strong impact of interaction energies on the porosity and pore connectivity of formed model aggregates.

[1] Totsche, K.U., Amelung, W., Gerzabek, M.H., Guggenberger; G., Klumpp, E., Knief, C., Lehndorff, E., Mikutta, R., Peth, S, Prechtel, A., Ray, N. & Kögel-Knabner, I. (accepted): Microaggregates in soils. *Journal of Plant Nutrition and Soil Science.*

[2] Witten, T. A. & Sander, L. M. (1983). Diffusion-limited aggregation. *Phys. Rev. B* 27, 5686-5697.