Laboratoire
Génie Civil
et géo-Environnement
Lille Nord de France

Séminaires du LGCgE

Conférence du Professeur Daniel Tunega

Institute of soil research de l'University of Natural Ressources ans Life Sciences de Vienne

Modeling of clays, soil organic materre (SOM) and clay-water-SOM interfaces

jeudi 13 février à 16h30

salle Atrium Bâtiment ESPRIT - Campus Cité scientifique Université de Lille à Villeneuve d'Ascq

Résumé

Soil condensed phases are mainly represented by two types of materials – soil organic matter (SOM), which is a result of decomposition of (bio)organic material, and soil minerals. Clay minerals such as kaolinite and smectite families predominate the clay-sized fraction of many soils. It is of utmost importance to understand interactions and formation of SOM-mineral aggregates at the molecular scale to explain e.g. sorption and buffer functions of soils and important stabilization mechanisms of SOM.

In this work we characterized the behavior of the kanolinite-water interface in the interaction with ions, glyphosate (one of the most used herbicide) and model aggregates of humic substances (HS) by means of classical molecular dynamics simulations. The models of HS aggregates were generated by a modeler developed in our group - Viena Soil-Organic-Matter Modeler (VSOMM).[1] Because of the nature of the modeled systems, interfacial phenomena play an important role in interface processes. Therefore, properties such as density profiles, polarization and dielectric properties, residence times, etc., are in the center of our interest. We observed that electrostatic phenomena seem to be the main driving force for adsorption at the clay-mineral interface, consequently leading to strong interactions with clay mineral surfaces characterized by hydrogen bonding and/or inner/outer surface complexation. This offers the possibility to deepen our understanding of the complex behavior of soil processes at an atomistic level, leading to explanations of phenomena at the macroscopic scale with application in environmental science and engineering.

[1] A. Sündermann, R. Solc, D. Tunega, G. Haberhauer, M.H. Gerzabek, C. Oostenbrink, Vienna soil organic matter modeler – Generating condensed-phase models of humic substances, *J. Mol. Graph. Model.* **62** (2015) 243-261. doi:10.1016/j.mgm.2015.10.007