EGU2020-7738
https://doi.org/10.5194/egusphere-egu2020-7738
EGU General Assembly 2020
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A Pore-Scale Reactive Transport Model Approach for Investigating the Effect of Soil Physical Properties on Biogeochemical Processes

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The vadose zone hosts a wide range of various microorganisms which provide different soil ecosystem services from nutrient cycling to biodegradation of harmful chemical substances. The efficiency of such in-situ biodegradation is influenced by different biotic and abiotic factors ranging from physical properties of the soil to the redox conditions controlled by the activity of the involved chemical compounds. One important feature of the soil system is the dynamical and simultaneous interplay of these factors, boosting or deteriorating the residing microbial community's abundance and/or activity and hence shaping biodegradation of vadose zone contaminants. Physical properties of porous media – e.g. the pore geometry, pore size distribution, connectivity as well as the water content – play a major role in enhancing or restricting the bioavailable concentration of contaminants and other reaction partners. Pore-scale phenomena have been shown to be considerably affecting the macro-scale processes, therefore a quantitative bottom-top approach of these mechanisms in situ is adamant. Hence it is of paramount importance to understand the effect of soil physical properties on microbial activity and biodegradation of carbon compounds in soil.

Pore scale reactive transport processes have a complex, nonlinear dependency on the aforementioned factors, which severely challenges the experimental and/or numerical investigation of biodegradation at in in-situ conditions. However, the recent technological advances, specifically the imaging techniques, have made it easier to study biological and microbial evolution in porous media, but there is still a need for putting all these information together. For this purpose, numerical methods would offer the possibility of simulating a variable/controllable water saturation conditions and considering water/air dynamics and advective and diffusive micro-scale transport of all components in both, air and water phase, in porous medium structures directly obtained from CT scanned samples. Up to now, such pore-sale model approaches considering also the fate of biogeochemically reactive compounds are scarce. In this work we propose a novel reactive transport modelling technique combining the pore-scale numerical characterization of water flow and solute transport in unsaturated porous media and of biogeochemical process. For a variably saturated porous system, the presented model approach is solving the Navier Stokes equation and scalar transport equations for any arbitrary geometry and is simulating the dynamics of biogeochemical processes with any degree of complexity. Simulations are compared to experimental data to assess the effect of soil physical properties on

the transport and degradation of contaminants in soil.