Predicting solute transport in structured soil using pore network models

Max Köhne, Hans-Jörg Vogel, and Steffen Schlüter
Helmholtz Centre for Environmental research - UFZ, Soil physics, Germany (max.koehne@ufz.de)

We evaluate a new approach for predicting solute transport through soil based on observable structural properties of the material. The methodology centres on X-ray micro computed tomography of a hierarchic suite of undisturbed soil samples (diameters 1, 5, 7.5, 16 cm) to identify the network of pores above 10 \(\mu\)m in diameter. The pore structure is quantified in terms of pore size distribution, interface area density, and connectivity. The pore size distribution and pore connectivity are employed to set up an equivalent pore network model (PNM) used for predicting the BTC of bromide (Br) and Brilliant Blue FCF (BB) at unsaturated, steady-state flux through undisturbed soil columns. For a structured loamy soil, the predictions of Br tracer breakthrough were within the variation observed in the column experiments. A similarly good prediction was obtained for Br breakthrough in a sandy soil column. Next, batch experiments were conducted for estimating sorption properties of BB. For predicting BB breakthrough, the average sorption distribution coefficient, \(k_d\), was considered in the model. The BB breakthrough observed in the loam was dominated by a large variation in sorption as expressed by the order-of-magnitude range in retardation factors. When the \(k_d\) from the batch test was used in the PNM, retardation was overestimated. By contrast, transport in the sandy soil column could be roughly predicted using the batch test \(k_d\). The prediction improved when applying a sorption correction function accounting for the deviation between measured interface area density distribution and its realization in the network model. Considering that the pore structure quantification and the transport model are both conceptual simplifications of the reality, the agreement between model results and data was excellent for Br tracer in both soils, while it was good for BB and the sandy soil. The results thus support the hypothesis that solute transport can be estimated based on a limited number of characteristics describing pore structure: the pore size distribution, the pore topology and the pore-solid interfacial density.