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Effect of pore-scale interfaces on dissolved chemical transport in unsaturated structured soil: a pore network model simulation

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The main obstacle for a reliable prediction of chemical displacement in soil is the inherent heterogeneity of the material which is structured at multiple scales. Soil structure invokes a heterogeneous flow regime depending on saturation and atmospheric boundary conditions. Additionally, the macroscopic transport pattern of dissolved chemicals is affected by their local interactions at interfaces between (macro)pores and the soil matrix, thereby enhancing dispersion and invoking retardation.

A pore network model was extended for assessing effects of soil structure on the transport of solutes, with focus on the contact intensity and sorption to interfaces. In the pore network model, the soil structure was quantified in terms of interfaces, pore size distribution, and topology. This information was derived using X-ray-micro-tomography of the porous structure of a Chernozem soil column sampled from the experimental field station Bad Lauchstädt (Germany).

Network model simulations were conducted to predict the water retention and conductivity functions and the transport of a tracer (bromide) and an adsorbed solute (Brilliant Blue FCF) at two different water saturations. Results of the model predictions were compared with corresponding experimental hydraulic and transport measurements and gave mostly satisfactory agreement. Next, the network model was used to study potential effects of the chemical heterogeneity of pore-matrix interfaces, as e.g. caused by the different mineral and organic constituents, on the retardation of reactive chemical. The non-uniform spatial distribution of interface adsorption properties had a considerable effect on the solute breakthrough curve. First results suggest that the network modelling approach can be seen as a step towards linking soil structure parameters with the reactivity of dissolved chemicals.