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Investigation of reactive transport with closed-flow column experiments and parallel factor analysis (PARAFAC) of fluorescence data

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The sorption of solutes and colloids to immobile sorbents results in the phenomenon of retardation. Besides the interactions at the sorbent-solution-interface, the sorption rate depends also on the spatial structure of the pore network (size distribution, connectivity, topology). Column experiments allow for the consideration of the structure and thus for a quantification of possible rate limitations. We focus on column experiments run in closed-flow mode. There, a typical oscillation in the "breakthrough" of solute concentration, which conveys additional information about the flow regime (dispersivity, water content, immobile water) as well as the effective interaction kinetics, can be observed. Another major feature of the closed flow design is the conservation of tracer mass inside the column setup. Therefore, the investigation of sorption characteristics can be simplified by using mass balances.
Our objective is to study the interaction between different solutes (conservative tracers, e.g., NaCl or LiBr and reactive tracers, e.g., acetate, oxalate and phenanthrene) and artificial porous media (composed of quartz, illite, goethite and charcoal in a well defined grain size distribution). The concentration-time profile of solutes is measured with non-consuming techniques (fluorescence spectroscopy or electrical conductivity measurements). PARAFAC analysis of fluorescence data is used for the quantification of aromatic compounds in complex background solutions. Interaction parameters obtained from breakthrough data are then used to quantify the availability of reactive mineral surfaces and effective rates of physical and chemical non-equilibrium processes. After the column experiments, the effect on the microtopology and mineral surfaces is investigated by atomic force microscopy and scanning electron microscopy. Recent multi-step tracer experiments allowed for the reconstruction of adsorption isotherms of oxalate and acetate on goethite.