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Reactive transport of Selenite and Strontium through a goethite coated sand column

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A sound understanding of the key mechanisms governing the mobility of contaminants in the environment is of primary importance. Goethite occurs in numerous natural settings as well as in potential host rocks for high level nuclear waste repositories as an accessory mineral.

A previously proposed CD-MUSIC type model for Se(IV) adsorption on goethite in the presence of Sr(II) [1] was found to be insufficient for simulating breakthrough curves (BTCs) in column experiments, in which Se(IV) and Sr(II) containing solutions were pumped through a goethite-coated sand packed column. The simulations of the BTCs improved when contributions from the quartz surface were included (i.e. assuming that goethite does not completely cover the quartz surface). The BET surface area (SSA) is corrected, based on a new approach [2], where the crystal habit of a model crystal, derived from TEM images, is used. Simulation of the static data with this SSA and associated face contributions and site densities, starting from proton related surface charge and subsequently Se(IV) and Sr adsorption to goethite, yielded a new set of parameters for the goethite model. These parameters and inclusion of a silica acid-base and strontium adsorption model resulted in improved simulation results. The partial coverage of the sand with goethite poses further challenges due to charge heterogeneities and overlapping of surface potentials. Also, the dissolution of quartz and re-adsorption of silicic acid may play a significant role [3], which will be implemented in the model.

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