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CRESCENDO: Development and testing of a new Charge Regulation Surface Complexation Model for interacting electric double layers

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Electric Double Layers (EDLs) develop at the interface of (mineral) surfaces and electrolyte solutions through surface (de-)protonation reactions, the adsorption of ions, and electrostatic effects. They consist of a Stern-layer of specifically adsorbed ions and a diffuse layer of mobile ions.[1]The implementation for the modeling of changes in surface chemistry caused by charge regulation (CR) effects of overlapping EDLs from multiple surfaces in current modeling approaches is very limited. Electrostatic interaction between surfaces is calculated by solving the Poisson-Boltzmann equation (PBE). As analytical solutions of the PBE only exist for simple geometries and electrolytes[2,3] it needs to be solved numerically. The new Python-based code combines a general chemical speciation code with an up to Three Plane Surface Complexation Model and a Finite Element solver for the PBE. It implements CR by calculating the chemical equilibrium of all involved surfaces simultaneously while including the effects of electrostatic interaction. The PBE solver was compared to analytical solutions and the chemical speciation code was benchmarked against a model of Am(III) sorption on quartz implemented in PHREEQC. CR test cases of parallel as well as perpendicular surfaces are presented. This new approach enables the investigation of charge regulation effects on various topics such as colloid stability, chemical speciation in nanoconfined spaces, and transport through nanoporous materials like clay[4] which can be relevant for a wide variety of research fields such as environmental and biological systems, cementitious materials, or natural and engineered barriers in nuclear waste repositories.

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