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# Incorporating surface phenomena into solute transport through compacted clays - Application of the Poisson–Nernst–Planck set of equations

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Surface phenomena in the clay pore space gain in relevance as the level of compaction increases and the dimensions of the space confined between clay layers shifts towards the range of nanometers. At such scales, solute transport can no longer be explained by concentration gradients alone. In fact, the electrical double layer (EDL) that develops in the neighborhood of the negatively charged clay surfaces can extend well into the aqueous phase, effectively constraining the space available to anions (an event known as anion exclusion) and, in general, distorting the spatial distribution of ionic species in solution. This can be addressed by solving the Poisson-Nernst-Planck (NPP) set of equations, which allows for the determination of the electric potential over the entire domain, along with the spatial distribution of the concentration of ionic species. Although this approach has been taken for some time in the field of Nanofluidic dynamics, it has largely been neglected in clay science.
In this context, the present work attempts to bridge the gap between Nanofluidic dynamics and clay science by proposing the simulation of multicomponent solute transport in compacted clays by means of the solution of the PNP set of the equations using a two-dimensional finite-element framework. Modeling procedures are presented in detail and then applied to a simple case reported in the literature (Van Loon et al., 2007). Numerical results were found to match experimental data more accurately than those obtained by other Donnan-based models over a wider range of dry densities. In light of this, it is then argued that the NPP set of equations can provide a more reliable basis for the incorporation of surface phenomena into the modeling of solute transport through compacted clays.