Multiscale modeling of electro-kinetic transport in porous materials

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The surface of many minerals is charged and so is the fluid in contact with them. This polarization of the mineral-fluid interface results in couplings between the solvent and ionic fluxes, the so-called electrokinetic effects. As an example, electro-osmosis generates a solvent flow under an applied electric field. In geophysics, the electro-seismic effect, by which an electromagnetic wave is generated from the motion of underground fluids under an applied acoustic wave, is exploited to determine the properties of geologic formations. Streaming potentials and electro-osmotic flows can be measured in the laboratory to characterize the properties of porous media.

From the modeling point of view, electrokinetic phenomena in porous materials are particularly challenging due to the variety of scales involved. These phenomena arise within the electric double-layer, where the fluid is locally charged, typically in the nanometer range, where interactions on the molecular scale also play an important role (ion specificity, slippage). On the pore scale, which may be from tens of nanometers to microns or more, viscous momentum diffusion drives the fluid away from the double-layer, even where the fluid is electrically neutral. Finally, a real material involves a complex pore network, so that heterogeneities on larger scales must also be taken into account. Of course, all these length scales are associated with increasingly long time scales, from picoseconds for the motion of water and ions near the surface to seconds or more for transport across a macroscopic sample.

These challenges can be addressed using a multiscale modeling approach. In this presentation, I will discuss results obtained using a combination of simulation techniques corresponding to complementary levels of description, namely: molecular dynamics [1,2], mesoscopic Lattice Boltzmann Electrokinetics [3,4,5] and Pore Network Models [6]. Their contributions to the understanding of electrokinetic phenomena will be illustrated on the case of clays.

[1] Rotenberg et al (2013), *Mol. Phys.* **111**, 827 [2] Botan et al (2013), *J. Phys. Chem. C* **117**, 978 [3] Pagonabarraga et al (2010), *Phys. Chem. Chem. Phys* **12**, 9566 [4] Rotenberg et al (2010), *Faraday Discussions* **144**, 223 [5] Obliger et al (2013), *Phys. Rev. E* **88**, 013019 [6] Obliger et al (2014), *Phys. Rev. E* **89**, 043013