

Molecular transport mechanisms in confined clays

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Understanding transport through clay pores is necessary in many contexts, such as groundwater hydrology, carbon dioxide sequestration or geological disposal of radioactive waste. As soon as we are interested in natural environment, an aqueous solution is present in the medium and will play a crucial role in structuration and transport of mobile species.

Molecular dynamics simulations allow to access adsorption properties at the surface of the clay layer. Ions and water molecules confined in clays show relative different structural and dynamical behaviors at the interface depending on the clay charge, its location and the nature of the ions. In small pores, the presence of the clay surfaces induces a slowing down of the mobile species, with diffusion mechanisms different from bulk aqueous solutions [1,2], which can be compared with neutron diffusion measurements. Coupling experiments and simulations is very useful to help to better understand the diffusion mechanisms in confined interlayer spaces on a large range of temperatures, as to test the validity of the force field which describes the intermolecular interactions used in the simulation.

In bigger pores where advection is not negligible, the pore-scale flow is usually described by the Navier-Stokes equation. However the validity of this continuous solvent equation can be questioned, especially in pores where the flow can be seriously influenced by the fluid interaction with the surface. In this case, non-equilibrium molecular dynamics (NEMD) simulations can be used to investigate the validity of continuous hydrodynamics in clay pores. The characteristics of hydrodynamic flows show that the Navier-Stokes equation can be used to predict simulated flow, as long as slip boundary conditions are taken into account at the solid/liquid interface [4,5]. Like in small interlayer spaces, these conditions depend on the charge of the clay, its location in the clay layer and the type of counterions present in the pore.

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