

Pore geofluid characterization using neutron scattering, adsorption measurements, and molecular modeling

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Fluid-solid interactions of pure and mixed geofluids confined in the narrow pores of earth materials play important roles in the uptake, mixing, storage, extraction, and transport of these fluids. Fluid-pore interactions play out at the molecular to microscopic levels, and include sorption, wetting, diffusion, and flow, all impacted by confinement effects. Fluid-solid interactions play out at the surfaces, and clays and porous silica have some of the largest surface areas of minerals. In addition, clay and silica fractions often show significant intergranular porosity, and swelling clays in hydrated state have appreciable pore volumes in interlayer pores. Therefore, clay-fluid interactions may control the properties of fluids in shale and other clay-rich rocks. I will discuss excess sorption, small angle scattering, and neutron diffraction data we have collected to gain insight into clay and silica interactions with noble gases, light hydrocarbons, water, and CO₂. This work aims at obtaining a basic understanding of the sorption capacity and fluid recovery amounts and rates of shales, and their dependence on shale composition, structure, and pore size distribution. Of great interest are the accessibilities of clay interlayer pore spaces, which contain large fractions of the clay and shale internal surfaces, to different fluids. The experimental data are interpreted to yield the mean fluid densities in the interlayer spaces, and their possible coordinations with the interlayer cations and their hydration shells. Quasielastic neutron scattering was used to assess mobility of pore confined water, hydrocarbons, and their mixtures. Molecular modeling provides detailed insights into sorption mechanisms and diffusion processes.

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