

Behavior of Water and Aqueous Solutions in Nanopore Systems

DAVID R. COLE¹ AND ALBERTO STRIOLO²

¹School of Earth Sciences, The Ohio State University,
Columbus, OH USA 43210 (cole.618@osu.edu)

²Department of Chemical Engineering, University College
London, London, UK (a.striolo@ucl.ac.uk)

A comprehensive understanding of the structure, dynamic, and reactivity of water at multiple length scales (molecular to macroscopic) over wide ranges of temperature, pressure, and composition is foundational to advances in quantifying geochemical processes involving mineral-fluid interfaces. Behavior of fluids in confined geometries (pores, fractures) typically differs from their bulk behavior in many ways due to the effects of large internal surfaces and geometrical confinement. Phase transitions (i.e., freezing and capillary condensation), sorption and wetting, and dynamical properties, including diffusion and relaxation, may be modified, with the strongest changes observed for pores < 50 nm. Factors influencing the structure and dynamics of confined fluids include the pore size and pore size distribution, the degree of pore connectivity, and the character of the liquid-surface interaction. The confining matrices of interest to earth sciences usually contain oxide structural units and thus are generally hydrophilic. The pore size distribution and the degree of porosity and interconnection vary greatly amongst porous matrices. Rocks typically possess irregular porous structures, whereas zeolites, and layered systems, e.g., clays, have high degrees of internal order. The richness and complexity of fluid behavior in confined geometries only underscores the need to adopt a multidisciplinary approach when quantifying this behavior regardless of the fluid type or nature of the porous medium. The properties of neutrons make them an ideal probe for comparing the properties of bulk fluids with those in confined geometries. Here we discuss fluids confined in materials such as silicas, aluminas, zeolites, and clays, emphasizing techniques that assess both structural modification and dynamical behavior such as small-angle (SANS) and quasielastic neutron scattering (QENS). Molecular dynamics (MD) simulations provide atomistic characterization of the confined fluid behavior as well as aid in the interpretation of the neutron scattering results. If properly calibrated and scaled, an atomistic to molecular-level understanding of fluid-solid interaction may provide quantitative insight into the behavior of systems at the macroscopic level.