Structure, dynamics and reactivity of fluids in confined geometries

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Hydrocarbons, aqueous solutions, and gaseous species (e.g. CO_2, CH_4) can occupy the pores or fractures of numerous types of complex heterogeneous solids. The size, distribution and connectivity of these confined geometries, the chemistry of the solid, the chemistry of the fluids and their physical properties collectively dictate how fluids migrate into and through these micro- and nano-environments, wet and ultimately react with the solid surfaces. Many solids are comprised of pore regimes ranging from large macropores at the millimeter scale to small micropores at the sub-micron and nanometer scale. Our current understanding of the rates and mechanisms of fluid and mass interaction within these multiporosity systems at the molecular scale is far less robust than we would like. We will provide an overview of the application of state-of-the-art experimental, analytical and computational tools to assess key features of the fluid-matrix interaction. The multidisciplinary approaches highlighted will include neutron scattering and NMR experiments, thermodynamic measurements and molecular-level simulations to quantitatively assess molecular properties of C-O-H fluids confined to well-characterized porous media, subjected to temperatures and pressures relevant to subsurface energy systems. These studies conducted in concert provide a fundamental understanding at the molecular level of how intrinsically different fluids behave in confined geometries compared to bulk systems.