

NMR Relaxation of Alkanes and Water in Nanoporous Shale Systems

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Classical theories of the Nuclear Magnetic Resonance relaxation, such as the Bloembergen-Purcell-Pound (BPP) theory, is based on simple assumptions of the molecule and its environment. This is inadequate for any complex fluid, reflected in the relaxation measurements of highly viscous fluids or fluids trapped in nanopores. This is particularly important in interpreting NMR logs of fluids in shale, where the rock matrix is dominated by nanopores. To this regard, we employ a novel technique to extract NMR relaxation data from molecular simulations, by probing the underlying relaxation mechanism. We use this to study various complex fluids, and fluids under nanoconfined shale system. In this talk, I will first present our work on alkanes in a polymer matrix system. We find, both experimentally and by simulation, that relaxation times decreases with increasing viscosity of the fluid. We also see that at high viscosities, there is the signature behavior of alkanes trapped in shale, i.e. high T1/T2 ratios and frequency dispersion for T1. We proceeded with simulations of alkanes in synthetic shale system that replicates the pore distribution of shale. The results were remarkably consistent with our previous observations with alkanes “trapped” in polymer matrix. I will conclude the talk with discussions on our current work on simulations of alkanes in realistic shale systems, which incorporates both confinement and chemistry of the system.