

Alkali Metal Cation Specific Effects at Calcite/Brine Interfaces for Wettability Alteration

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Abstract. SmartWater flooding involves the injection of water with favorable chemistry to improve oil recovery in carbonates. The interactions between dissolved ions in aqueous solutions and rock surfaces play an important role to govern wettability, which can be altered towards water-wet conditions thereby leading to increased oil production. Nevertheless, the role of specific ions and valency still holds some ambiguity, especially with carbonate rocks that are generally more reactive than sandstones. This study aims to systematically investigate the interactions between calcite and alkali metal cations (Li^+ , Na^+ and K^+) using zeta potential measurements and molecular dynamics (MD) simulation. Calcite was used to represent rock substrate as it constitutes the most stable polymorph of calcium carbonate besides being the dominant mineralogical composition of carbonate reservoirs. Calcite dissolution at atmospheric CO_2 levels and laboratory conditions has been shown to have a negligible effect on alkali metal chloride solutions speciation at ionic strengths of 0.025, 0.05, 0.075 and 0.1 mol/kgw. The zeta potential results showed that the calcite/brine slip plane charge becomes more negative with smaller radii ($\text{Li}^+ < \text{Na}^+ < \text{K}^+$) indicating an inverse relation between ionic radii and the extent of adsorption. The same trend was captured in the MD simulation; these findings are consistent with the free energy of solvation for these ions.