

Comparing Classical Force Fields for Aqueous NaCl Solutions at Elevated Temperatures and Pressures

Katie Maerzke^{C, S}, Lara Patel and Robert Currier
Los Alamos National Laboratory, Los Alamos, NM, U.S.A.
kmaerzke@lanl.gov

Meeting the ever-increasing demand for fresh water will ultimately require desalination, which at present remains an expensive endeavor. One promising new approach is supercritical desalination, which can be co-mingled with the extraction of valuable co-products as a cost offset. The properties of water vary dramatically with temperature and density. Near ambient conditions, water acts as a strong dielectric to screen ionic charges. However, the dielectric constant decreases significantly near and above the critical point, which can be exploited to control solubility. Given the high temperatures and pressures, molecular simulation is a valuable technique for examining the behavior of ions in high temperature and supercritical water. However, the degree of accuracy one can expect from classical force fields under these conditions is unclear. We have thus undertaken a parameter study for NaCl in water, comparing several salt and water models to experimental data (where available) and to each other. We will present a comparison of structural properties, such as the degree of ion aggregation and extent of hydrogen bonding, as well as thermophysical properties, such as pressure-composition diagrams.