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Molecular dynamics insights of NaCl-bearing fluids at deep-Earth conditions

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Aqueous fluids transport metals and control their complexation and deposition at high temperatures and pressures in the deep Earth. The composition of these fluids is chemically complex, yet sodium chloride (NaCl) is one of the major components. Understanding certain physicochemical properties of NaCl brines (equation-of-state, ion association, electrical conductivity, and dielectric constant) is important in order to predict speciation, thermodynamic properties, and stability of metals at high T-P conditions. Currently, there is a lack of physicochemical data at high temperature, pressure, and molality due to difficulties in experimental measurement at these conditions.

A powerful tool for predicting physical and chemical properties of aqueous systems is molecular dynamics, a computational method which uses classical mechanics to simulate chemical systems. Through the implementation of force fields with appropriate benchmarking, this method computes molecular trajectories allowing for the calculation of properties such as equation-of-state, dipole moment, diffusion, and structural behaviour.

In this study, we used force field molecular dynamics to provide insights into equation-of-state, ion association, electrical conductivity, and the dielectric constant of NaCl-bearing fluids at a wide range of T-P-X (up to 1000ºC, 60kbar). We implemented a newly developed NaCl force field[1] in combination with SPC/Fw water[2] to study brines near the supercritical point of water, with additional benchmarking results at ambient conditions. Our results complement previous theoretical and experimental studies and provide insights into the physicochemical properties of brines at high T-P-X, allowing for improvement to interpretations of geophysical data.

[1] Loche, Steinbrunner, Friedowitz, Netz & Bonthuis (2021), *J. Phys. Chem. B* 125 (30), 8581–8587.

[2] Wu, Tepper & Voth (2006), *J. Chem. Phys.* 124 (2), 024503.