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Comparing Molecular Dynamics Models for Electrolyte Solutions in Nanochannels[1] JONATHAN LEE, JEREMY TEMPLETON, Sandia National Laboratories — In electrolyte modelling, it is common to simplify the solvent using the three-component model (3CM), i.e. a single-site, chargeless Lennard-Jones atom as the solvent component. To account for the dielectric nature of typical solvents, a relative permittivity value is applied to all Coulombic interactions, thus weakening ion-ion interactions as if each ion is surrounded by a solvation shell. Fluid Density Functional Theory, Monte Carlo simulation, and molecular dynamics (MD) simulation all commonly employ the 3CM to facilitate calculations, but the consequences are not well characterized. We used MD to compare the 3CM electrolyte to a molecular solvent model (MSM) where the solvent is a three-site H_2O) molecule. Special care was taken to compare cases with the same thermodynamic state by having a quantifiable reference state, and cases covered a range of applied surface charge in a nanochannel configuration. At a glance, the two models give qualitatively similar density profiles. However, we find that many profile features, physical quantities such as electric field and potential, as well as ionic packing structure near the surface evolve quite differently as the load is varied.

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