A Low Mach Number Fluctuating Hydrodynamics Model For Ionic Liquids

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We present a new mesoscale model for ionic liquids based on a low Mach number fluctuating hydrodynamics formulation for multicomponent charged species. The low Mach number approach eliminates sound waves from the fully compressible equations leading to a computationally efficient incompressible formulation. The model uses a Gibbs free energy functional that includes enthalpy of mixing, interfacial energy, and electrostatic contributions. These lead to a new fourth-order term in the mass equations and a reversible stress in the momentum equations. We calibrate our model using parameters for [DMPI+][F6P-], an extensively-studied room temperature ionic liquid (RTIL), and numerically demonstrate the formation of mesoscopic structuring at equilibrium in two and three dimensions. In simulations with electrode boundaries the measured double layer capacitance decreases with voltage, in agreement with theoretical predictions and experimental measurements for RTILs. We present a shear electroosmosis example to demonstrate that the methodology can be used to model electrokinetic flows. We are currently exploring three-dimensional effects and new formulations for the free energy.