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Numerical modeling of ultrasonic cavitation in ionic liquids

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— Ionic liquids have favorable properties for sonochemistry applications in which the high temperatures and pressures achieved by cavitation bubbles are important drivers of chemical processes. Two different numerical models are presented to simulate ultrasonic cavitation in ionic liquids, each with different capabilities and physical assumptions. A model based on a compressible form of the Rayleigh-Plesset equation (RPE) simulates ultrasonic cavitation of a spherical bubble with a homogeneous interior, incorporating evaporation and condensation at the bubble surface, and temperature-varying thermodynamic properties in the interior. A second, more computationally intensive model of a spherical bubble uses the finite element method (FEM) and accounts for spatial variations in pressure and temperature throughout the flow domain. This model provides insight into heat transfer across the bubble surface and throughout the bubble interior and exterior. Parametric studies are presented for sonochemistry applications involving ionic liquids as a solvent, examining a range of realistic ionic liquid properties and initial conditions to determine their effect on temperature and pressure. Results from the two models are presented for parametric variations including viscosity, thermal conductivity, water content of the ionic liquid solvent, acoustic frequency, and initial bubble pressure. An additional study performed with the FEM model examines thermal penetration into the surrounding ionic liquid during bubble oscillation. The results suggest the prospect of tuning ionic liquid properties for specific applications.

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