Modeling of ion transport in ether-based liquid membranes

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To accelerate the development of liquid ion-selective barriers based on ethers, we compare the all-atom force fields GAFF, OPLS-AA with charge correction 1.14*CM1A (OPLS-AA/CM1A), CHARMM version 36 (CHARMM36), and COMPASS for diisopropyl ether (DIPE) to determine the most appropriate model for further molecular dynamics simulations of liquid membranes. Utilizing the selected force fields, we calculate the density and shear viscosity of DIPE across a temperature range of 243–333 K. Furthermore, we use CHARMM36 with mTIP3P water model and COMPASS with its own water model to evaluate the mutual solubility and interfacial tension between DIPE and water, estimate the partition coefficients of ethanol in DIPE + Ethanol + Water systems. Based on our comparative study, we conclude that CHARMM36 is the most suitable force field for modeling ether-based liquid membranes. These results were published in [1]. Subsequently, the CHARMM36 force field was used to model solutions of lithium and chloride ions in water and DIPE. Transport properties of ions, such as mobility and diffusion coefficients, and structural properties, including pair correlation functions, were investigated. The diffusion coefficients and ion mobility were estimated based on the steady-state ion current under an applied constant external electric field. The study was conducted for solutions with ion concentrations of 0.01 and 0.1 M and at various strengths of the external field.

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