

DIFFUSION AROMATIC HYDROCARBONS IN IONIC BY MD SIMULATION

Atamas N.A., Bardik V.Yu., Gavryshenko D.A.

¹*National Taras Shevchenko University of Kyiv, Physics Department,
2 Glushkov Ave., Kyiv 03124, Ukraine
e-mail : atamasphys@mail.univ.kiev.ua*

Ionic liquids (ILs) have been extensively studied as replacements to sulfolane in the separation of aromatics from alkanes. The employment of ILs could reduce energy requirements and operating costs of the aromatic extraction unit as a result of their nonvolatile character. However, the ILs studied so far have shown mass-based aromatic distribution ratios lower than the sulfolane values, which would increase the solvent-to-feed ratio in the extractor.

The MD method was applied using a modified DL_POLY_4.05 with a time step of 2 fs for study of structure and diffusion aromatic hydrocarbons in IL (dimethyl-imidazolium chloride-dmim⁺/Cl⁻) at T=400K. In the calculations cations, anions, and atoms forming the molecules of the added substance (hydrocarbons : benzene, toluene, phenol , anisole and c-hexane) were treated as solid charged model systems with a fixed geometry. Analysis of the data allowed to establish: (1) The solvation effect in systems dmim⁺/Cl⁻ - non-polar solute molecules (benzene, c-hexane) has qualitatively similar to the behavior of the hydrophobic hydration of aromatic solute molecules in liquids like water. Based on the data obtained from MSD and VAF the different diffusion mechanisms of nonpolar solute molecules in IL were determined. (2) The solvation effect in systems ionic-liquid (dmim⁺/Cl⁻) - polar solute molecules (toluene, phenol, anisole) has qualitatively similar to the behavior of the hydrophobic hydration in liquids like water too. Based on the data obtained from MSD and VAF the different diffusion mechanisms of hydrocarbons solute molecules in IL were determined.