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Molecular Simulation of the Effect of Imidazolium-Based Ionic Liquids on the Water/Toluene Interface

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Crude oil is a complex mixture of organic compounds which are conventionally categorized as saturates, aromatics, asphaltene and resins based on their polarity and solubility. Aromatics, in particular, comprise a large portion of many light, medium and heavy oils therefore it is important to understand their interfacial properties with water and surfactants in the context of enhanced oil recovery. In this work, we explore the effect of imidazolium-based ionic liquids on water/toluene interface using molecular dynamics (MD) simulation. Imidazolium ionic liquids are cationic organic compounds comprised of a heterocyclic aromatic head with a saturated aliphatic chain. The MD simulations were based on classical OPLS and SPC/E force fields with the leap-frog numerical integration scheme, 1.2 nm cut-off for Lennard-Jones potential and particle mesh Ewald summation for the electrostatic interactions. The interfacial tension (IFT) for pure water and toluene was found to be 36.09 mN/m at 300 K and 1 bar which is close to the experimental value of 35 mN/m. Adding imidazolium chloride at a surface coverage of two molecules for every square nanometer slightly reduced the IFT to 32.71 mN/m for the butyl chain. For Ionic liquids with octyl and dodecyl chains, the IFT of water/toluene has been significantly reduced by approximately a factor of 2 and 8, respectively. Calculations of the interaction energy between the two phases shows that imidazolium cations with longer chains interact more strongly with Toluene, thereby effectively reducing the IFT. Furthermore, density profiles across the axial-direction perpendicular to the interface shows that the ionic liquids with longer alkyl chain partition more toward the interface whereas the butyl imidazolium have a low surface excess and are not as surface active as the octyl and dodecyl imidazolium. Therefore, imidazolium interacts with toluene more via its alkyl chain and the association between the toluene and the imidazolium aromatic head is limited at the water/toluene interface.

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References

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Primary author: ALSHAMMARI, Salem

Co-authors: ABU-AL-SAUD, Moataz (Saudi Aramco); Dr ABDEL-AZEIM, Safwat (King Fahd University of Petroleum and Minerals)

Presenter: ABU-AL-SAUD, Moataz (Saudi Aramco)

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