

Sodium Chloride Behavior at Oil/Water Interfaces

Nahid Pour Khiabani¹, Alireza Bahramian¹, Mohammad Reza Ejtehad², Peyman Pourafshary¹,
Madjid Soltani³, Pu Chen³

¹*Institute of Petroleum Engineering, University of Tehran, Iran;* ²*Department of Physics, Sharif University of Technology, Tehran, Iran* ³*Department of Chemical Engineering, Waterloo, Ontario, Canada*

The interface formed between an aqueous salt solution and a hydrophobic liquid has been investigated using molecular dynamics simulations, to compare ion distribution and interfacial properties. Hexane has been selected as the hydrophobic liquid. Hydrophilic liquid is an aqueous solution of NaCl to analyze the behavior of monovalent anions and cations at hexane/water interface. The interfacial tension of hexane/pure water interface was found to be 60 mN/m, in reasonable agreement with the experimental value of 54 mN/m at the temperature of 25° and the pressure of 1 atm. Our simulations also show the increase in hexane/water interfacial tension with the increase of salt concentration consistent with experimental data. Density profiles of hexane, water, anions and cations reveal the formation of a double layer, so that the anions are closer to the interface than cations. Radial distribution function (RDF) studies show a noticeable difference between the interfacial and bulk RDFs, so that the interfacial RDFs have a higher first hydration shell peak than the bulk RDFs.