**From Solvation Free Energy to Wettability Alteration by Low Salinity Water Flooding in Sandstone Oil Reservoirs: A Molecular Dynamics Simulation Approach**

Hadi Ansari 1[[1]](#footnote-1)\*, Amin Rezaei 2

1 Faculty of Petroleum and Chemical Engineering, Science and Research Branch, Islamic Azad University, Tehran, Iran

2 Department of Chemical and Petroleum Engineering, Sharif University of Technology, Tehran, Iran

**Abstract**

Nowadays, the application of the low salinity water flooding (LSWF) technique to improve oil recovery from hydrocarbon reservoirs has grabbed the attention of many scientists due to its cost-effectiveness and environmentally friendly nature. Acquiring the underlying mechanisms of this method for enhanced oil recovery purposes is a complicated process that requires a good understanding of the reservoir rock mineralogy and fluid properties. Primarily, LSWF is prone to alter the rock surface wettability. However, there are controversial debates about the effects of LSWF on changing the wettability of rock surfaces (mainly composed of quartz minerals) in a rock/oil/brine system. To be more specific in understanding the characteristics of the rock/oil/brine system at the atomic level, classical molecular dynamics simulations (MDS) in the presence of n-decane, as the synthetic oil, sandstone rock, and brine with different salt concentrations were performed. To this end, the indirect contact angle values were calculated using the solvation free energy (SFE), obtained from MDS approach, along with the Zisman plot (provided by KRUSS Co.). The results showed that there is a direct correlation between the SFE value and contact angle. Reciprocally, an inverse relationship was observed between ion concentration and the contact angle so that increasing ion concentration leads to decreasing contact angle and vice versa.

1. \* Corresponding author, Email: hadi.ansari@srbiau.ac.ir [↑](#footnote-ref-1)