Factors Affecting Water/Oil Interfacial Tension as Identified by Molecular Simulations

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The interfacial tension (IFT) of a fluid-fluid interface is a well-defined property, which plays a very important role in a wide range of applications and processes. When low IFT is desired, surface active compounds (*e.g.* surfactants) can be added to the system. Numerous attempts have been made to relate the IFT reduction due to such compounds and their molecular structure at the interface. However, IFT is controlled by the interplay of many different factors such as temperature, pressure, salinity, as well as the presence of surfactants, which make it difficult to predict IFT as those conditions change. In this study, by conducting molecular dynamics simulations we found that the interfacial entropy is a more general descriptor to capture IFT, especially when surfactants are added. Related to this observation, surfactants that yield more disordered interfacial films (*e.g.* with flexible and/or unsaturated tails) reduce the water-oil IFT more effectively than surfactants which yield highly ordered interfacial films. The more surfactants are added to the system, the more entropy contributes to lower the IFT. Also, the stronger the interactions between surfactant headgroups and counter ions and water, the less IFT is reduced. Our results contribute to better understanding of some of the factors that control the IFT and could have important practical implications in industrial applications ranging from the design of cosmetics and detergents to surfactant formulations for addressing various challenges in the oil and gas sector.