Molecular Simulations of Surfactants for Water/CO_2 and Water/Hydrocarbon Interfaces

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Carbon dioxide has proven to be very effective for enhanced oil recovery (EOR) purposes, but common techniques such as alternating water/CO_2 injection require large CO_2 sources to be financially feasible. However, a similar effect can be achieved via an implicit mechanism based on dual-action emulsifying agents (surfactants). Surfactants will be used to create an emulsion-like mixture with water and CO_2 which gets injected into a hydrocarbon reservoir, where the surfactants dual-affinity will cause a transition to a hydrocarbon/water emulsion. Thus, trigger a release of CO_2 inside the reservoir while simultaneously improve recovery of hydrocarbons. This concept effectively combines safe storage of carbon dioxide with EOR, and will be financially feasible even for small CO_2 sources. The proposed concept relies on pinpointing surfactant candidates with affinity towards both the water/CO_2 as well as water/hydrocarbon interfaces. To investigate the potential of the approach, we have used molecular dynamics (MD) simulations. Using an all-atomic description of the involved components, we have performed MD simulations of various surfactant structures in water/CO_2 and water/hydrocarbon liquid interfacial systems. In addition to existing surfactants, we have also modified their molecular structures, and performed MD simulations with the modified structures for comparison. Our results strongly suggest that organic morpholine structures exhibit the desired dual-affinity and adsorb at both types of interfaces. Analysis of the interfacial regions has been performed to investigate the specific impact of each surfactant structure, including; broadening of interfacial region, structure of the interfaces, composition, and molecular orientation. Our study also showed how small modifications to the molecular structure can alter the surfactants' interfacial behavior, providing potentially useful insight for design of surfactants.