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Experimental Investigation and Molecular Dynamics Analysis of the Fluid-Fluid Interactions between Binary Surfactant Systems for EOR

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This work aims to explore the properties and interactions between binary surfactant systems due to their ability to form mixed micelles with lower interfacial tension (IFT). The focus is on determining the synergistic or antagonistic behaviors of these systems for effective application in enhanced oil recovery (EOR) in carbonate oil fields. Our study employed a methodology comprising experimental analysis, mathematical modeling, and molecular dynamics simulations. In the experimental study, we examined eight individual surfactants and six binary surfactant systems at various ratios to determine their critical micelle concentrations (CMCs), using reservoir oil and performing experiments at reservoir conditions. Then, Rubingh's Regular Solution Theory (RST) was applied to evaluate interactions within the binary surfactant mixtures. Finally, using molecular dynamics simulations, we characterized the microscopic interactions to comprehend how hydrophilic and hydrophobic parts of the surfactants interact with surrounding media, and how they self-assemble into aggregates such as micelles or bilayers. The key findings of our work showed that the occurrence of synergism or antagonism in lowering the CMC of binary surfactant mixtures depend on both the concentration of the individual surfactant and the type of surfactant used. Nevertheless, we noted a prevalent synergistic phenomenon in all binary surfactant systems, notably influenced by the concentration of the non-ionic surfactant. Increased concentrations of non-ionic surfactants notably enhanced synergistic interactions, fostering lowered CMC values when combined with anionic, cationic, and zwitterionic surfactants. On the other hand, an excessive concentration of cationic surfactants demonstrated relatively 'weak' synergistic effects, attributed to their comparatively smaller hydrophobic tail. Moreover, the formation of mixed micelles in binary surfactant systems led to a more negative free energy of micellization, thereby achieving synergistic effects between surfactants and resulting in lower CMC values. This emphasizes the crucial role of surfactant concentration in achieving synergistic outcomes within mixed systems. Generally, binary surfactant systems demonstrated lower CMC values compared to single surfactants, suggesting the potential for their use at lower concentrations to achieve desired interfacial and recovery outcomes, thereby reducing operational costs.

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References

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