SALT CONCENTRATION EFFECTS ON THE MORPHOLOGY OF MICELLAR SOLUTIONS OF IONIC SURFACTANTS AND THEIR MIXTURES WITH ZWITTERIONIC CO-SURFACTANTS

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ABSTRACT

Liquid formulations based on anionic surfactants find extensive use in personal care products. In the absence of salt, surfactants organize into spherical or tiny rod-like micelles, and their zero-shear viscosity is close to that of water. Adding small amounts of salt increases the zero-shear viscosity by several orders of magnitude, approaching a peak value beyond which adding more salt causes a decrease in the viscosity [1]. Salt alters the shape of the micelles and increases their size resulting in what is known as wormlike micelles. To design formulations with predefined properties, a fundamental understanding of how the solution composition affects the micelle microstructure is thus needed, together with the latter's connection with the rheological behavior of the solutions. However, a quantitative connection between the microstructure morphology and the solution composition is currently missing.

The present work addresses the impact of salt concentration on the morphology of micelles formed by anionic surfactants and their mixtures with zwitterionic co-surfactants. We use the sodium laurylether sulfate as a model anionic surfactant and the cocamidopropyl betaine as a zwitterionic co-surfactant. We employ a hierarchical simulation approach already implemented with great success to predict the morphology of anionic surfactant solutions under salt-free conditions [2,3].

Our simulations show that, in the absence of salt or at tiny salt concentrations, small spherical micelles are formed. By further increasing the salt concentration, cylindrical micelles are formed, which upon adding even more salt aggregate into giant wormlike micelles with a contour length up to several tens nanometers, in agreement with experimental observations [1]. Moreover, adding zwitterionic co-surfactants increases the cohesion between surfactants. Detailed results from these highly-demanding simulations will be presented and compared one-to-one to experimental measurements.

Overall, our computational approach allows the accurate prediction of micelle size, micelle shape, and salt curves for industrially-relevant formulations of surfactants over a broad spectrum of conditions. What is more important is that information from these molecular-level simulations about the morphological features of the giant micelles formed at high salt concentrations in the solution can be used to parametrize a Brownian Dynamics code that addresses the complex rheological behavior of these systems.

KEYWORDS: Micellar solutions, self-assembly, anionic surfactants, simulations

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