Predicting the size of surfactant micelles incorporating hydrophobic additives – quantitative model vs experimental data

Joyce Lemmer [a], *Karen Edler* [b], *Jyoti Gupta* [c], *Nicholas Brownbill* [c], *Gokhan Topcu* [c], *Adam Squires* [a]

a Department of Chemistry, University of Bath, Claverton Down, Bath BA2 7AY, United Kingdom
b Department of Chemistry, Lund University, Lund 221 00, Sweden
c Unilever R&D Port Sunlight, Quarry Road East, Bebington Wirral CH63 3JW, United Kingdom

jl4390@bath.ac.uk

This is a study that predicts the size of spherical surfactant micelles in the presence of hydrophobic additives.

Surfactants are known to play a vital part in many processes in both fundamental and applied science. These compounds can self-assemble under aqueous conditions into molecular aggregates called micelles. [1] Due to their structure, micelles are used in a range of different applications, such as in detergency, pharmaceuticals and nanotechnology, where they can act as simple delivery systems for small hydrophobic additives. Depending on the additive, these molecules can alter the physical properties of the surfactant, including their phase behaviour, surface tension and viscosity, and thus the final formulations' performance. [2] It is therefore of great importance to understand and predict the effects of additives on the self-assembly of these systems.

We present a quantitative geometric model that can predict the size of spherical surfactant micelles in the presence of hydrophobic additives. This model was applied to predict the size of sodium dodecyl sulfate (SDS) micelles in binary mixtures (surfactant/water) and their swelling in ternary mixtures (surfactant/n-decane/water), as a function of their surfactant/additive/water volume fractions. Molecular parameters were extracted from the d-spacing of more ordered phases (lamellar and hexagonal). Results show that the experimental values are in good agreement with the model values, limited to predictions up to the maximum solubility concentration of the hydrophobic additive (MAC). This approach not only bridges theoretical modelling with experimental results but also provides a practical tool to estimate the effect of additives on the surfactant micelles more accurately, which in turn would help in the improvement of formulations for future surfactant-based products.

Keywords:
Surfactants, Micelles

References:

[1] Abbott, S. (2017). *Surfactant Science: Principles and Practice,* DEStech Publications, Incorporated
[2] Rosen, M. J. and Kunjappu, J. T. (2012). *Surfactants and Interfacial Phenomena* . John Wiley & Sons, Inc.