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Determining the micellar composition of sulfobetaine surfactants through small-angle neutron scattering and molecular dynamics simulations

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Sulfobetaines are zwitterionic surfactants with peculiar properties such as high foam stability, temperature resistance and salt tolerance (SiTu et al., 2017). Sulfobetaines are widely used in body care products and kitchen detergents. Despite their widespread use, micelle self-assembly and packing are not explored. In this work, we study hydroxyl sultaines to develop high-performance and environmentally friendly fluorine-free firefighting foam due to their suitability to withstand harsh conditions. This study combines small-angle neutron scattering (SANS) and molecular dynamics (MD) simulations to investigate the micellar architecture of sulfobetaine surfactants.

SANS experiments were conducted for three lauramidopropyl-derived zwitterionic surfactants in different temperatures and concentrations to probe the micellar structure in solution. Analysis revealed the presence of ellipsoidal micelle with a well-defined core-shell morphology. This allowed the determination of optimal headgroup area, volume of core, aggregation number and packing parameter. These experimental findings are complemented by atomistic MD simulations. We made the models of preformed micelles of various sizes and subjected the simulation trajectories to analyse the micelle size, eccentricity, solvent-accessible surface area and self-diffusion. Simulated radii and eccentricity of the micelles showed the fluctuations in the major and minor of the ellipsoid's axes confirming the ellipsoidal model fitted by SANS. Exploring the internal composition of micelle gives fair knowledge about surfactant packing in solution and this knowledge will be used to make better firefighting agents out of sulfobetaine precursors.

References

SiTu, W.X., Lu, H.M., Ruan, C.Y., Zhang, L., Zhu, Y., & Zhang, L. (2017). Effect of polymer on dynamic interfacial tensions of sulfobetaine solutions. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 533, 231-240. https://doi.org/https://doi.org/10.1016/j.colsurfa.2017.09.006

Topics

Chemistry and Crystallography

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