Structural Properties of Ionic Surfactants using a SAFT-γ Mie Force Field in Molecular Simulation

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Surfactants are molecules with both, hydrophobic and hydrophilic constituents. Due to this amphipathic structure, they are subject to various phenomena such as the lowering of interfacial tension and the formation of microstructures (e.g. bilayers and micelles). The focus of this work are anionic surfactants, which are widely used in in the consumer product industry. The determination of phase behaviour, i.e. the prediction of microstructures dependent on concentration, temperature and pressure, as well as the critical micelle concentration (cmc), the concentration of surfactant required to start the formation of micelles, are key properties of interest. These are important to assess the effectiveness of a surfactants for a particular task and also to facilitate its production. The determination of phase behaviour and cmc for an aqueous sodium dodedcyl sulfate (SDS) solution is therefore at the centre of this work. Molecular simulation is a powerful tool for the prediction of the aforementioned relevant physical quantities from a molecular model, thereby deepening our understanding of which molecular motifs are critical to the desired behaviour and reducing reliance on resource intensive experiments. However, for the time- and length-scales required to determine the quantities of interest, commonly used atomistic or united-atom models reach the limits of computational tractability. Therefore, coarse grained molecular models are used to extend system sizes and simulation times [1, 2]. In the current work, the SAFT γ-MIE equation of state [3], which was recently extended to electrolytes [4], is used to parametrise the nonbonded interactions of an aqueous SDS solution utilising a large set of experimental data. Combined with bonded interactions, parametrised via iterative-Boltzmann inversion (IBI) [5], a complete molecular model is obtained. The coarse grain model is used to efficiently predict the cmc and size distribution of micelles in aqueous solution using molecular dynamics simulation. Furthermore, the consideration of experimental data across different state points results in good transferability across temperature and concentration ranges.

References

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