Simulation Studies of Coarse Grained Surfactant Models

Samantha Sanders* and Athanassios Z. Panagiotopoulos
Department of Chemical Engineering, Princeton University

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Surfactants are used for a wide range of industrial and biological applications. Composed of a hydrophilic head group and a hydrophobic tail group, they self-assemble into various structures in aqueous solutions. Atomistic models cannot reach the necessary time and length scales for self-assembly in dilute solutions. Therefore, various coarse grained models have been developed. A recent group of coarse grained models provides semi-quantitative information. However, these models have not been tested on their ability to reproduce experimentally measured critical micelle concentrations (cmc's). In this work, we analyze the MARTINI model [1, 2] for its ability to reproduce the cmc's of the zwitterionic surfactant dodecylphosphocholine (DPC) and an ethoxylated non-ionic surfactant, C8E4. We obtain molecular dynamics trajectories on the order of microseconds at multiple temperatures allowing the determination of cmc's and aggregate size distributions. Our results suggest that the model underpredicts the critical micelle concentrations by 1-2 orders of magnitude. While the monomer surfactant concentration reaches equilibrium, the aggregate size distribution does not reach equilibrium. We have compared our molecular dynamics-based method to a semi-grand canonical Monte Carlo method for calculating the critical micelle concentration [3] and found our results to be in agreement. Finally, we have examined the impact of using replica exchange molecular dynamics. From each of these studies, we determine aspects of the model in need of refinement in order to create quantitative, transferrable models for surfactant self-assembly.

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[2] S.J. Marrink, H. J. Risselada, S. Yefimov, D. P. Tieleman, and A. H. de Vries, *J. Phys. Chem. B* 111, 27 (2007).
[3] R. Pool and P. Bolhuis, *J .Phys. Chem. B* 109, 14 (2005).