

Supporting Document

Influences of Surfactant and Nanoparticle Assembly on Effective Interfacial Tensions

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Although the manuscript focuses on experimental evaluation of surfactant and nanoparticle assembly on effective interfacial tensions, a small portion of simulation work is included to provide complementary information on why tetraethylene glycol monododecyl ether ($C_{12}E_4$) and tetraethylene glycol monotetradecyl ether ($C_{14}E_4$) fail to decrease the interfacial tensions of water-TCE interfaces. This supporting document briefly addresses the potential effect of simulation methods and cutoff distances.

First, we have evaluated the possible effect of the cutoff distance in the particle-mesh Ewald (PME) method for the $C_{12}E_4$ surfactant, as shown in Figure S1. All simulations, regardless of the cutoff distance, have shown that the $C_{12}E_4$ molecules do not equilibrate at the water-TCE interfaces but disperse in the TCE bulk phase, which provide complementary information to the experimental observation.

Second, we have applied both the cutoff method and the PME method in simulations of the SDS surfactant. Figures S2a-c compare the density profiles from the cutoff method with different cutoff distances, 9 Å, 12 Å, and 14 Å, respectively. The density profiles from the PME method with a cutoff distance of 12 Å are shown in Figure S2d. All simulations have shown that the SDS molecules equilibrate at the water-TCE interfaces, although the density profiles using the PME method appear to be superior to those using the cutoff method.

In summary, all simulations with different cutoff distances in the PME method and the cutoff method and have shown that the $C_{12}E_4$ molecules disperse in the bulk TCE phase at the equilibrium whereas the SDS molecules tend to equilibrate at the water-TCE interfaces.

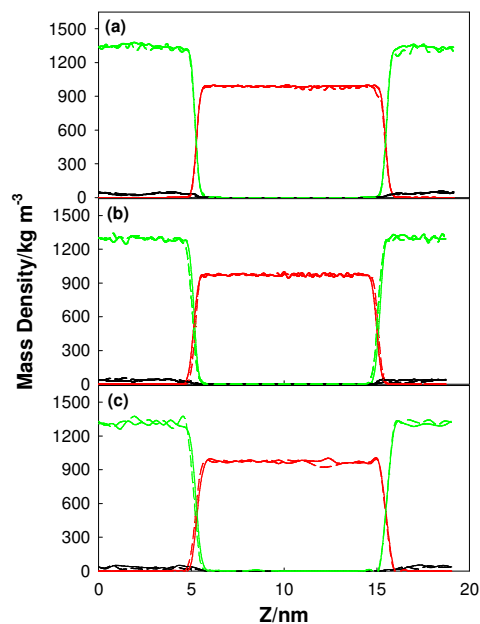


Figure S1. Mass density profiles of System A5 using the PME method with different cutoff distances. (a), (b), and (c) use cutoff distances of 10 Å, 12 Å, and 14 Å, respectively. The C₁₂E₄, SPC, and TCE are represented in black, red and green, respectively. Two parallel runs were performed on each system.

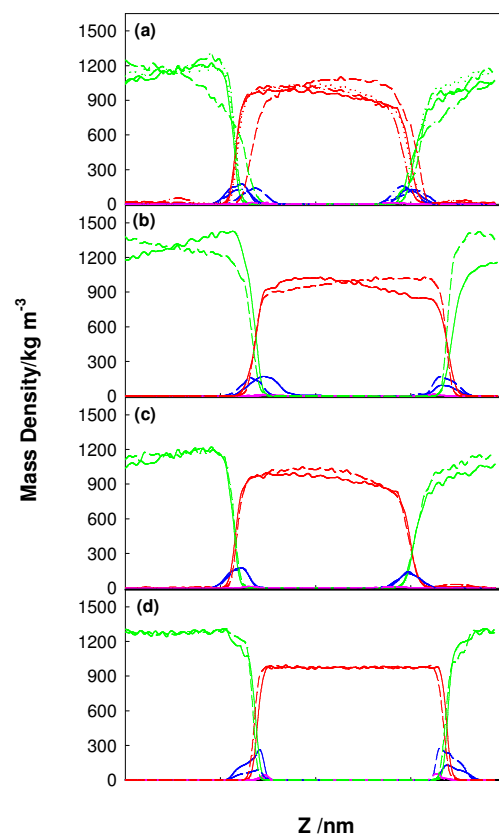


Figure S2. Mass density profiles of System C5 using the cutoff and the PME method. (a)-(c) use the cutoff method with cutoff distances of 10 Å, 12 Å, and 14 Å, respectively, and (d) uses the PME method with a cutoff distance of 12 Å. The SDS, Na⁺, SPC, and TCE are represented in blue, pink, red and green, respectively. Two parallel runs were performed on each system except four runs in (a).