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Presentation Title	Transport properties of micelles and monomers in surfactant solutions via Monte Carlo and molecular dynamics simulations
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Abstract

Transport properties of micelles and monomers in surfactant solutions via Monte Carlo and molecular dynamics simulations

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In contrast to the nonionic micelles, a diffusivity of ionic micelles can be a non-monotonic function of the total surfactant concentration [1,2]. The results on the diffusivity in micellar solutions are usually obtained by dynamic light scattering experiments. Interpretation of the experimental data is typically based on a bimodal approximation for the distribution of surfactant aggregates which presumes that there are only monomers and stable micelles of certain size. More reliable is picture of dispersed aggregates, and here the methods of molecular modeling allowing one to look at individual aggregates and analyze the distribution of their sizes can be very helpful. The diffusivity of ionic micelles and all monomers in aqueous solution is simulated via Monte Car lo and molecular dynamics methods as a function of aggregation number and total surfactant concentration. A molecular dynamics of aqueous solution of sodium dodecyl sulphate (SDS) at normal conditions is carried out using MDynaMix package [3]. An all-atom representation of SDS and solvent has been employed, CHARMM36 force field [4] and TIPS3P water model [5] are used. Within a Monte Carlo approach, a system of charged hard spheres of different sizes in a dielectric continuum is simulated in order to study an equilibrium distribution of negatively charged micelles and monovalent positive counterions. A distribution of sizes of the spheres corresponds to a typical distribution of stable ionic surfactant aggregates in aggregation numbers. The result of the simulations is a dependence of the micelle diffusivity on micelle aggregation number, surfactant concentration and concentration of added electrolyte. This dependence is compared with the experimental results and some theoretical models.

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