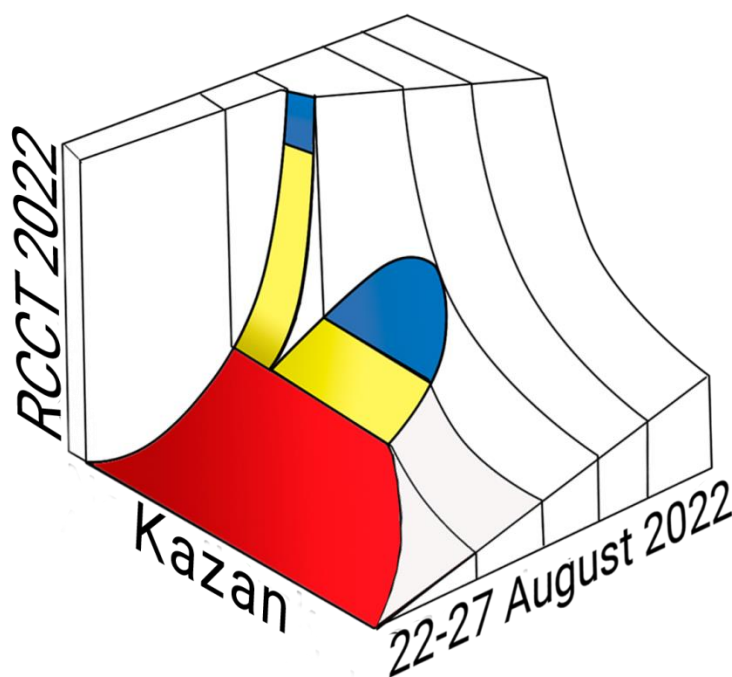# XXIII International Conference on Chemical Thermodynamics in Russia

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BOOK OF ABSTRACTS

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MOLECULAR THERMODYNAMIC MODELING OF AGGREGATION AND TRASMEMBRANE POTENTIAL FOR VESICLES FORMED BY IONIC SURFACTANT MIXTURES

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Vesicles are spherical bilayer membranes which are widely used as nanoreactors and containers for application in micellar catalysis and drug delivery [1]. Vesicular aggregates commonly self-assemble from mixtures of cationic with anionic surfactants in solution [2, 3, 4]. The molecular thermodynamic aggregation models [2, 5, 6] aim at predicting properties of the self-assembled aggregates based on the molecular parameters of surfactants. The majority of molecular-thermodynamic models of aggregation employ the Poisson-Boltzmann theory to describe the electrostatics assuming electroneutrality of the vesicle's interior. This implies no drop of the electrical potential across the membrane of the vesicle. However, the transmembrane potential is very important because it is the driving force for the transfer of mobile ions across the membranes.

In this work, we discuss the version of the classical aggregation model [5] that leads to an analytical expression for the transmembrane potential [6] within the linearized Poisson–Boltzmann theory. This expression reflects the dependence of the transmembrane potential on the parameters of the vesicle (including its curvature and charge) and on the solution salinity. Maxima or minima of the transmembrane potential may appear in response to variation of salinity. We show that adding salt to solution may lead to the reversal of the sign of the transmembrane potential, and demonstrate that a vesicle brought to equilibrium with an acidic environment may hold an alkaline solution in its interior.

We predict aggregation behavior for catanionic mixtures of classical surfactants (sodium alkylsulfates with alkyltrimethylammonium bromides and sodium dodecylbenzenesulfonate with 1-hexadecyl-3-methylimidazolium chloride) that form vesicles, including distributions of the aggregates over their size and shape (spherical and rodlike micelles, and vesicles), the aggregate's composition and the micelle-to-vesicle transitions. The molecular parameters of surfactants have been taken from the literature [5]. Comparison with SANS and cryo-TEM data [3, 4] shows that the vesicles with the radius of less than 30 nm are reasonably predicted by the model. The predicted values of the electrical potential in the electrical double layer around the vesicles formed by cetyltrimethylammonium bromide with sodium octylsulfate agree with experimental data for the zeta potential [2].

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