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BOOK OF ABSTRACTS

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Influence of additives in Triton X solutions on micellar properties and solute partitioning for the design of bioprocesses

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Abstract

Micellar systems can be used in various technical application such as solubilizing agents, drug delivery systems or material in the thermal separation processes like cloud point extraction (CPE). Aqueous nonionic surfactant solutions can form two phase systems above the cloud point temperature (CPT) and can be considered as alternative solvent for extraction processes. Due to their aqueous environment and their generally low salt content, these systems are of interest in particular for bioprocesses. For the design of such processes, the partition coefficient between both phases dependent on pH-value, phase composition and additive concentration needs to be known. An extended understanding of the partition behavior can be received from such structural information as micelle shape and size and micelle composition, especially in case of mixed surfactant solutions. Furthermore, the physicochemical properties (viscosity, surface tension etc.) of the system are important parameters for the identification of the operating window.
In the present work, the partition behavior of solutes in aqueous Triton X solutions in presence of different additives (salt, other surfactant) was under investigation. Due to its low CPT, Triton X-114 can be regarded as suitable surfactant for a biocatalytic extractive process using the hydrolysis of penicillin G to 6-aminopenicillianic acid and phenylacetic acid [1]. For the design of this process, the partition coefficients of the reactants as well as the liquid-liquid equilibrium were measured dependent on pH-value, reactant and salt (NaCl and K_2HPO_4/KH_2PO_4) concentrations. An identification of suitable operating parameters was supported by a study of the physicochemical properties, namely density, surface tension and viscosity.
Moreover, this study was conducted to improve the understanding of solute distribution in micellar systems to increase a quality of predictions of the micelle-water partition behavior. Therefore, partition coefficients of model solutes (with varying functional groups) in aqueous Triton X-100 solution and mixtures of Triton X-100 and nonionic surfactant Brij 35 were determined by micellar liquid chromatography. A composition of the mixed micelles as a function of the Triton X-100/Brij 35 ratio were determined both theoretically within the regular solution approach and experimentally by NMR diffusometry [2]. The critical micelle concentrations received from tensiometry measurements showed non-ideal behavior of the mixed micelles. Additionally, the micelle size data were obtained from dynamic light scattering experiments, these results are important findings to predict micelle-water partition coefficients using thermodynamic models like COSMOmic, an extension of COSMO-RS [3]. The consecutive predictions showed a good agreement with the experimental partition coefficient values; also in case of the mixed micelles with different composition.

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