Partition coefficients of ionizable solutes in aqueous micellar two-phase systems

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ABSTRACT

The potential of micellar cloud point systems for extraction processes has been demonstrated for a broad range of different applications. The extraction is based on the phenomenon that aqueous non-ionic surfactant solutions split into two phases if the temperature is increased beyond a certain temperature, the so called cloud point temperature (CPT). Recently, aqueous micellar two-phase systems have been implemented in a counter current extraction. However, almost equally important for large scale applications is the recovery of the solute from micellar solutions, which remains a serious concern considering micellar cloud point systems as alternative to conventional solvents. In conventional solvent extraction processes the influence of the pH on the partitioning of ionizable solutes is an important parameter to control the extraction and back extraction efficiency. However, the partitioning of ionizable solutes such as organic acids and bases in micellar two-phase systems has not been studied so far. In this work the partitioning of various ionizable solutes including phenolic as well as pharmaceutical active compounds has been investigated. Lipophilicity profiles of all solutes were analyzed for the system Triton X-114/water in a pH range between 2 and 12. Further, the influence of temperature, solute concentration, as well as different salt concentrations on the partitioning of charged solutes was investigated. Experimental results are verified by means of predicted values using the thermodynamic model COSMO-RS. The results reveal that COSMO-RS can be applied to predict the partitioning of ionizable solutes in micellar biphasic systems, when the phase behavior of the pure surfactant is known.

Based on these data optimal strategies for large scale micellar extraction processes are proposed and validated by means of a continuous pilot plant micellar extraction column.

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1. Introduction

Surfactant solutions have several advantages compared to conventional solvents, therefore growing interest is paid to these systems for a variety of applications, such as drug delivery systems [1,2], biosepartions [3,4], and waste water treatment [5–7]. Due to the amphiphilic nature of surfactant molecules, they form micellar aggregates in aqueous solution, whereas the hydrophilic head group is directed towards the aqueous bulk phase and the hydrophobic tail towards the center of the aggregates. Aqueous non-ionic surfactant solutions are known for their unique phase separation behavior upon altering conditions such as temperature [8]. The corresponding temperature is referred to as cloud point temperature (CPT). The phase diagram of the nonionic surfactant Triton X-114 (TX114) is shown in Fig. 1. At low surfactant concentration and temperatures a single isotropic solution can be observed (denoted by I). Increasing the temperature, the solution separates into two liquid phases (defined by 2L): a surfactant lean phase (also referred to as aqueous phase) which has very similar