Predicting Liquid-Liquid Equilibria for Water Desalination Using a Free Energy-Based Approach

Prashanth Chandran and Jindal Shah [C, S]
School of Chemical Engineering, Oklahoma State University, Stillwater, OK, U.S.A.
jindal.shah@okstate.edu

Conventional desalination technologies include energy-intensive distillation or pressure driven membrane processes. Recently, directional solvent extraction (DSE) has emerged as a viable low-temperature and low-energy alternative which utilizes a solvent capable of selectively dissolving water by rejecting the salt ions and at the same time having negligible solubility in water phase. The dissolved water is then extracted either by heating or cooling the water-solvent phase. Thus far, the proof-of-concept has been demonstrated with decanoic acid for which the extraction efficiency, defined as amount of pure water produced per 100 kg of solvent, is only 0.5 % suggesting that improvements are needed. This can be achieved by *in-silico* screening of a large number of molecular structures that can extract substantially higher amounts of water than decanoic acid. Success of such a screening critically depends on the ability to calculate solubility of water in solvents. As is widely known, liquid-liquid equilibria (LLE) calculations from molecular simulations continue to remain challenging due to the challenges associated with the transfer of molecules between two dense phases. In this presentation, we will describe the development of a novel molecular simulation methodology based on computing the fugacity of water as a function of concentration to calculate the extent of water dissolution in a range of solvents. First, the applicability of the LLE method is shown considering that the solubility of the solvent in water is negligible. The calculated solubilities are shown to give good agreement with experimental data for carboxylic acids with six to ten alkyl chain lengths over a range of temperatures. This method is also extended and demonstrated for systems exhibiting substantial mutual solubility unlike directional solvents and water. In addition, the structural properties elucidating the role of the hydrogen bonding interactions between water and directional solvents governing the solubility will be presented.