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Molecular Modeling and Prediction of the Physicochemical Properties of Polyols in Aqueous Solution

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Abstract : Roquette Frères is a producer of plant-based ingredients that employs many processes to extract relevant molecules and often transforms them through chemical and physical processes to create desired ingredients with specific functionalities. In this context, Roquette encounters numerous multi-component complex systems in their processes, including fibers, proteins, and carbohydrates, in an aqueous environment. To develop, control, and optimize both new and old processes, Roquette aims to develop new in silico tools. Currently, Roquette uses process modelling tools which include specific thermodynamic models and is willing to develop computational methodologies such as molecular dynamics simulations to gain insights into the complex interactions in such complex media, and especially hydrogen bonding interactions. The issue at hand concerns aqueous mixtures of polyols with high dry matter content. The polyols mannitol and sorbitol molecules are diastereoisomers that have nearly identical chemical structures but very different physicochemical properties: for example, the solubility of sorbitol in water is 2.5 kg/kg of water, while mannitol has a solubility of 0.25 kg/kg of water at 25°C. Therefore, predicting liquid-solid equilibrium properties in this case requires sophisticated solution models that cannot be based solely on chemical group contributions, knowing that for mannitol and sorbitol, the chemical constitutive groups are the same. Recognizing the significance of solvation phenomena in polyols, the GePEB (Chemical Engineering, Applied Thermodynamics, and Biosystems) team at Institut Pascal has developed the COSMO-UCA model, which has the structural advantage of using quantum mechanics tools to predict formation and phase equilibrium properties. In this work, we use molecular dynamics simulations to elucidate the behavior of polyols in aqueous solution. Specifically, we employ simulations to compute essential metrics such as radial distribution functions and hydrogen bond autocorrelation functions. Our findings illuminate a fundamental contrast: sorbitol and mannitol exhibit disparate hydrogen bond lifetimes within aqueous environments. This observation serves as a cornerstone in elucidating the divergent physicochemical properties inherent to each compound, shedding light on the nuanced interplay between their molecular structures and water interactions. We also present a methodology to predict the physicochemical properties of complex solutions, taking as sole input the three-dimensional structure of the molecules in the medium. Finally, by developing knowledge models, we represent some physicochemical properties of aqueous solutions of sorbitol and mannitol.

Keywords : COSMO models, hydrogen bond, molecular dynamics, thermodynamics
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