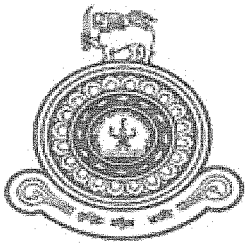

Theoretical Investigations of the Interactions Between Water and Nonylphenolethoxylate Surfactants

by

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Abstract

Surfactants are chemical substances which are widely used in industrial applications. The surface tension of water is affected by the addition of "surface active agents" or surfactants. Nonyl phenolethoxylates are surfactants which are commonly known as Tergitol NP surfactants . The molecular properties of nonylphenolethoxylate surfactants vary with the number of ethoxylate units in the molecule and are classified according to the number of ethoxylate units in the molecule. As an example Tergitol NP 10 contains 10 ethoxylate units in its molecule. These are widely used in paint industry and detergent industry. Hydrophilic lypophilic balance (HLB) is the key parameter in which formulators focussed their attention when studying these surfactants. Even if HLB values of surfactants are close enough to each other , the expected results cannot be obtained by replacing one with the other. This has been a very serious problem to formulators, because they have to carry out lots of trial and error testings to findout equivalents for a particular surfactant in a particular formulation. A comprehensive investigation of the nonylphenolethoxylate molecules has been carried out computationally at the abinitio level of theory to determine the interaction between nonylphenolethoxylate molecules and water by varying the number of ethoxylate units in the molecules. Therefore this research was designed to interpret the interactions of surfactants with water by using molecular properties such as hydrogen bond distance between water molecules and surfactant molecules , entropy change of emulsification, and surface tension of water after interacting with surfactants, by means of Gibbs free energy change of emulsification. Ability of emulsification varies along the surfactant series due to the responses given by them for interaction with water. According to the results obtained , it is clear that Tergitol NP 15 is the best emulsifier among the surfactants studied in this research project and by incorporating this surfactant to a particular formula, optimum properties for emulsification can be achieved and it leads to a better final product. It was revealed that this kind of computational study is useful prior to laboratory bench work to narrow down trial and error methods , which spends more money , time and energy, because these studies make provisions to compare the molecular properties of interested surfactants. Further, this study can be applied to many areas where surfactants play a key role in product formulations.