Abstract No: MP-04 **Multidisciplinary Research**

Computational investigation of the structural and thermodynamic properties of nonylphenol ethoxylate surfactants

B. D. S. Narthani and D. R. Pandithavidana*

Department of Chemistry, Faculty of Science,
University of Kelaniya, Sri Lanka
**Email: dinesh@kln.ac.lk*

The word "sufactant" has originated from the three words "surface active agents." Surfactants are compounds that have potential to lower the surface tension (or interfacial tension) between two liquids or between a liquid and a solid. Nonylphenol ethoxylates (NPEs) are a group of non-ionic surfactants commonly known as Tergitol NP surfactants. Nonylphenol ethoxylates are classified according to the number of ethoxylate units in the hydrophilic chain. The properties of the nonylphenol ethoxylates differ with the number of ethoxylate units in the molecule. The hydrophilic–lipophilic-balance (HLB value) is the key parameter that the surfactant formulates are focused on when studying the properties of non-ionic surfactants. Even though the HLB values of two surfactants are equal or close enough to each other, the expected properties cannot be obtained by replacing one surfactant with another one. This issue leads to the necessity to carry out many trial and error tests to identify the equivalent surfactants in industrial applications.

To address this issue, a comprehensive investigation of the nonylphenol ethoxylate molecules was carried out computationally at B3LYP level of theory using 6-311G basis set in Linux version of Gaussian 09 computer software package. The aqueous phase investigation focused on deducing the interactions between nonylphenol ethoxylates and water with extending the chain length of ethoxylate part, branching the nonyl hydrocarbon chain and varying the substituent position (-ortho, -meta and -para) of nonylphenol ethoxylate molecules. To interpret the interactions of nonylphenol ethoxylate molecules with water, molecular properties such as Gibbs free energy changes of solvation (ΔG_{solv}) in aqueous medium, molecular dipole moments and hydrogen bond lengths between surfactant molecules and water molecules were investigated.

The more negative values (-46.62 to -116.88 kJ/mol) of the solvation Gibbs free energy (ΔG_{solv}) indicated that stability of the NPEs in aqueous medium increases with the extension of the length of ethoxylate chain (4 to 16 ethoxylate units). The substituent position and the branching of the nonyl-hydrocarbon chain have not caused a change in Gibbs free energy of solvation significantly. Although electrical dipole moment of NPEs in aqueous medium varied with the position of the substituents, it was not affected by branching patterns of nonyl hydrocarbon group. Computationally simulated UV-Visible spectra of NPEs revealed the absorption maximum of NPEs (λ_{max}) was independent of ethoxylate chain length. UV-Visible spectra generated from selected molecules of NPEs confirmed that absorption maximum (λ_{max}) of the surfactant species was significantly affected by the change in position of substituents.

Keywords: Hydrophilic-lipophilic-balance (HLB), Nonylphenol ethoxylates ,