Abstract No: 772 ***Natural Sciences***

A THEORETICAL STUDY ON THE STABILITY OF DESIGNED MICROEMULSIONS

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Emulsion stability is one of the most important factors for the industrial and commercial applications of microemulsions. Emulsions can show kinetic or thermodynamic stability, depending mainly on the concentration of surfactants (emulsifiers) which stabilize the oil/water interface. The nominal surface excess concentration of surfactants needed to stabilize emulsion droplets is valuable information for designing and optimizing the composition of microemulsion systems. However, the efficiency and effectiveness of many surfactants in stabilizing oil/water interfaces is yet to be characterized. Here we study the stability of water-in-triolein microemulsions stabilized by Span80® surfactants, using molecular dynamics computer simulations. Prior to carrying out simulations, a coarse grained model for triolein was developed, extending the SDK coarse grained force field, allowing efficient simulation of relevant time scales and system sizes. The developed model accurately predicts triolein/water, triolein/air interfacial tensions. The model was used to carry out a series of molecular dynamics simulations varying the Span80® concentration at a triolein/water interface while measuring the change in interfacial tension. We show, that the area per surfactant required to obtain a tensionless triolein/water interface is ~50 $Å^2$ per surfactant. The stability of an emulsion droplet at this area per surfactant was confirmed, and furthermore, the spontaneous deformation of the droplet from spherical shape was observed for higher surface concentration of surfactants, using large scale simulations. The results obtained are applicable for many micro emulsion related applications, particularly water-in-olive oil emulsions. The major components of olive oil are triglycerides with oleic and palmitic chains, hence the triolein-water results can be used to guide the design of olive oil/water systems. These are particularly attractive candidates for topical skin creams and drug delivery systems due to the biocompatibility of olive oil, water and Span80®. Furthermore, because the parameters of the developed model are transferable further studies on a wide range of triglycerides are possible in the future.