From molecules to macrophases I: linking MD to fluid phase boundary predictions

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This project is part of an initiative to understand the behaviour of complex fluids involving surfactants using a multiscale modelling approach. This particular proposal centres on the problem of determining and ultimately predicting the viscosity of the phases, while a second linked proposal (“From molecules to macrophases II: Structural properties of ionic surfactant solutions”) focuses on the effect that ionic interactions have on phase diagrams in polymers.

In this project you will quantify, via large-scale coarse-grained molecular dynamics simulation, the capabilities of the SAFT-\(\gamma\) force field [1] to predict viscosities of complex fluid mixtures involving water, surfactants and oils. These mixtures will inevitably form mesophases (liquid crystalline structures such as micelles, vesicles, lamella) which will affect noticeably the viscous properties of the mixture. Knowledge of the phase boundaries is crucial in establishing the pathways for production and application of these mixtures, which are commonplace in the personal healthcare industry.

The ultimate aim of this project is to link molecular simulation with a macroscopic equation of state (SAFT) to map the boundaries and contours of phase behaviour and predict macroscopically observed process variables such as densities and viscosities. This will involve an exploration of the accuracy and limitations of the models to reproduce transport properties, in particular the diffusion and viscosity both in the bulk fluid range and in the dense liquid crystalline phases. We have evidence that the SAFT models provide quantitative descriptions for small molecules but have only briefly explored the quality of the representation for polymers, surfactants and systems with mesophases.

This project is a collaboration with our industry partner Proctor & Gamble and is fully-funded for Home and EU students. Technical and scientific enquiries may be directed to Prof Erich Muller (e.muller@imperial.ac.uk). General admissions enquiries should be directed to the TSM-CDT Senior Administrator, Ms Miranda Smith (miranda.smith@imperial.ac.uk).