METHODS FOR INVESTIGATING DISSOLUTION IN SURFACTANT SOLUTIONS

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Surfactants are present in many everyday products such as detergents and shampoos. Under certain conditions, surfactants will aggregate into different structures in solution. These different structures alter the rheology of the solution, and the exact structure formed is concentration dependant. This poses an interesting situation in which the rheology changes as the material dissolves. This research uses different simulation techniques to investigate both equilibrium phase behaviour, as well as the dissolution process. Most research focuses on understanding equilibrium behaviour, and non-equilibrium processes have been much less studied and are not as well understood.

Small scale modelling of the ‘clustering’ behaviour of surfactant molecules in solution helps us to understand the effects of the small scale on the rheology of the material. This poster will focus on the use of Lattice Monte Carlo (LMC) and Dissipative Particle Dynamics (DPD) methods. Both methods model molecules as a chain of 'beads'. LMC confines these beads to a lattice structure, whereas DPD is an off-lattice mesoscopic simulation technique which involves a set of particles moving in continuous space. While LMC can only be used to study the equilibrium behaviour of solutions, DPD can be used to study the dissolution process as well. This poster will compare the two methods, and show how DPD can be used to study the movement of surfactant molecules into an aqueous solution.

Incorporating small scale dissolution phenomena into large scale models, for example via multi-scale CFD approaches, is challenging and has received little attention in the literature. This is largely due to challenges capturing small scale phenomenon in a large scale simulation. One of the aims of this research is to investigate the feasibility of a coupled DPD-CFD model. This poster will discuss how such a model is implemented, and outline how a DPD-CFD model could work.

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