

Coarse-Grained Modelling of Particle-Stabilised Fluid Interfaces Using GENERIC and Simulations

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There is much interest in anisotropic particles adsorbed onto fluid-fluid interfaces in the context of self-assembly, surface rheology of particle-stabilised interfaces, e.g. Pickering emulsions as well as active nematics. We are interested in surface rheology, when the fluid-fluid interface has a microstructure formed by the anisotropic particles, a so-called complex interface. As a first approximation, we model anisotropic particles by hard ellipsoids and neglect capillary interactions. Non-equilibrium thermodynamic frameworks are a promising route to developing models of mechanical behaviour for many varied systems. The particular framework we use called GENERIC consists of four building blocks, which are functions of the state variables of the system we want to describe. The GENERIC building blocks are the energy, entropy, Poisson matrix and friction matrix, which combine to give a thermodynamically consistent, closed set of equations describing the whole system. We employ computer simulations and theoretical calculations for a system of hard ellipsoids confined to a plane in order to help guide the model development and extract functional forms of the building blocks. Using these, we construct a model to describe the rheology of fluid-fluid interfaces with adsorbed anisotropic particles.