Shear Viscosity of Binary Mixtures Using Molecular Dynamics and Stochastic Rotation Dynamics

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Understanding the link between microscopic properties and macroscopic behavior is one of the main challenges in colloidal science. A key quantity of interest is the shear viscosity, where the interplay between concentration, effective interactions, shape of the colloid, and hydrodynamics, can result in a complex behavior even for the simplest systems. Using computer simulations, we explore the shear viscosity of binary mixtures of colloidal suspensions. Due to the large colloid-solvent size ratio in systems of interest (e.g. calcium carbonate nanoparticles or cement C-S-H aggregates of 10-100 nm suspended in water), full atomistic simulations are ruled out and here we focus on mesoscopic simulations. We model the solvent using the stochastic rotation dynamics (SRD) approach [1], a method that includes thermal fluctuations and hydrodynamic interactions. SRD particles and colloids are coupled through stochastic collisions and we compute the shear viscosity using reverse nonequilibrium molecular dynamics, which allows the investigation of shear rate dependent transport properties. We show that the shear viscosity has a strong dependence on the velocity gradient of the colloid suspension with the suspension featuring both shear thinning and shear thickening regimes. For suspensions involving a bimodal size distribution of spheres, we find a reduction on the shear viscosity with respect to pure suspensions, validating predictions from previous theoretical work [2,3]. We highlight in our work the importance of the shear rate dependence on the viscosity of the binary mixture and the need to include these effects in the modelling of the rheological response of the suspension.

References:

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