More accurate predictions of ferrofluids' rheology

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Motivation

Ferrofluids have attracted considerable attention in the recent years, as their field-controlled physical properties has led to numerous applications, as well as in material science as in medical field [1,2]. Thus, modelling and simulating ferrofluid properties is an important stake to improve the comprehension of the macroscopic behaviour of ferrofluids, as well as to provide new tools so as to ease the development of new applications.

Models

Most of the ferrofluids simulations are performed using Molecular or Brownian Dynamics. Such simulations are able to predict macroscopic quantities (for instance, the magnetoviscous effect has been calculated in [3] for various concentrations and interaction strengths), or microstructural organization (structure factor, clusters…).
However, actual simulations regard ferrofluids as "perfect" magnetic suspensions, and may neglect some experimental important parameters, such as the wide size dispersion of magnetite particles. Moreover, the hydrodynamic interactions between moving particles are ignored.

Simulation of the hydrodynamic interactions

Brownian dynamics simulations are performed on a system containing 300 particles. At each time-step δt, the many-body interactions are computed according to the Rotne-Prager tensor. The difficulty arises from the need to uncorrelate the random motion of the particles. A method inspired from the polymer simulation has been employed, reducing the computational effort to $O(N^{2.25})$ [4].

For comparison purposes, another method has been employed, based on the calculation of the mobility matrix μ.
Once the equilibrium is reached, structural quantities, individual and global diffusion coefficients are calculated. The mean structural state of the simulation box is then compared to experimental data, obtained by SAXS and XPCS analysis [5].
Finally, the influence of the hydrodynamics interactions is investigated on a fluid submitted to a plane Couette flow, for various concentrations of particles and shear rates.

Polydispersity

To model real polydisperse ferrofluids, while keeping significant statistical data, a system containing small and large particles is studied. Following the work of Wang [6], our bidisperse particles have a radius ratio R_{small}/R_{big} set to 0.6. The other relevant simulation parameters correspond to usual ferrofluids ($\lambda \sim 1$, $\varphi = 1\% \sim 10\%$), while a variation in the fraction of small particles reveals a sharp modification of the state of the simulated fluid (cf. fig. 1).

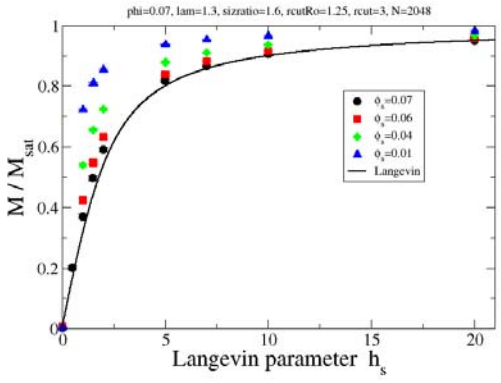

Figure 1: Magnetization of a bidisperse ferrofluid, for various radius ratio R_{small}/R_{large}. $\varphi = 7\%$, $\lambda = 1.3$.

To go further, predictions on the magnetoviscous effect of a simulation involving both bidispersity and many-body hydrodynamic interaction have been confronted to experimental results.

References

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