MICRORHEOLOGY SIMULATIONS USING SMOOTHED DISSIPATIVE PARTICLE DYNAMICS

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Microrheology is an experimental technique which allows one to obtain rheological properties of complex fluids. In these experiments, the movement of a colloidal particle inside a fluid is observed. From the diffusion of the particle, the viscoelastic properties of the surrounding medium fluid are inferred through a generalized Stokes-Einstein relation [1] [2]. Microrheology has comparative advantages with respect to traditional rheology: it allows using tiny quantities of fluids, the measurements are local and a broader frequency range can be investigated.

Despite its frequent use, there are still open questions about this technique, for example, the validity of the generalized Stokes-Einstein equation, or the influence of other colloidal particles on the diffusive motion of a single test particle. A simulation model able to address this type of problems should be very useful.

A computational technique suitable for this task should be able to model viscoelastic fluids with thermal fluctuations interacting with embedded rigid inclusions. The model we propose here [3] is a variation of the Smoothed Dissipative Particle Dynamics (SDPD) model [4], where a conformation tensor is used to reproduce the elastic behaviour of the fluid. As in the original SDPD model, we resort to the GENERIC formalism [5] to obtain thermodynamic consistency. The resulting equations conserve linear momentum and energy and fulfil the Second Law of Thermodynamics. In addition, thermal fluctuations are introduced in a natural way through the Fluctuation-Dissipation theorem and scale automatically with the resolution of the simulation [6]. The discrete equations obtained can be understood as a discretization of the equations of the Oldroyd-B model with thermal noise consistently incorporated.

The rigid colloidal particles moving through the viscoelastic matrix are modelled using frozen boundary SDPD particles filling the internal domain [7]. In order to assess the accuracy of the model in describing complex viscoelastic fluids under standard rheometric conditions, a simple small amplitude oscillatory flow (SAOS) will be simulated and the results compared with the theory. Furthermore, rheological properties will be evaluated also under simulated 'microrheological conditions' and the results discussed.

[1] Mason and Weitz, Phys. Rev. Lett. 74, 1250 (1995).
[2] Waigh, Rep. Prog. Phys. 68, 685 (2005).
[3] Vázquez-Quesada, Ellero and Español, J. Chem. Phys. 130, 034901 (2009).
[4] Español and Revenga, Phys. Rev. E 67, 026705 (2003).
[5] Ötinger and Grmela, Phys. Rev. E 56, 6633 (1997).
[6] Vázquez-Quesada, Ellero and Español, Phys. Rev. E 79, 056707 (2009).
[7] Bian, Litvinov, Ellero, Adams, in preparation