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MESOSCOPIC SIMULATIONS OF POLYMERIC SYSTEMS BY RESPONSIVE PARTICLE DYNAMICS

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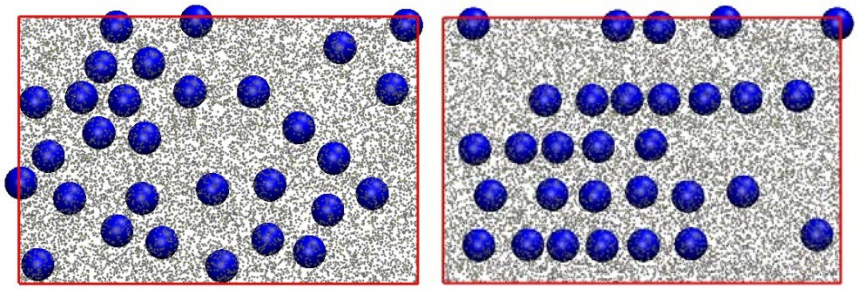
We have developed Responsive Particle Dynamics (RaPiD) to efficiently simulate the non-Newtonian flow behaviour of polymeric systems at the mesoscopic level. In RaPiD, each polymer is simulated as a single particle performing an extended Brownian motion. The conservative interactions between the particles are modeled by a free-energy functional based on the local polymeric density, e.g. the well-known Flory-Huggins theory. While this soft potential provides an adequate description of the thermodynamics behaviour of the system, it misses out on a key feature of polymer dynamics, namely the entanglements of the polymers. The formation and release of entanglements creates a memory effect on the mesoscopic level that is responsible for the visco-elastic flow behaviour on the macroscopic level. Hence, the slow relaxation dynamics of the (dis-)entanglements is modeled in RaPiD by introducing non-conservative interactions between particle pairs, by means of internal coordinates that qualitatively represent the degree of entanglement of two neighbouring polymers. The slow Brownian dynamics of these internal coordinates endows the simulated system with a transient memory of its past, and thereby creates a model with visco-elastic flow characteristics. The thermodynamic properties of the system are not affected by this altered dynamics.

In this presentation, we will show how the coarse-grained RaPiD approach can be used to describe the flow behaviour of various shear-thinning fluids. As an example, we discuss the behaviour of colloidal particles dissolved in two distinct visco-elastic fluids, representing a solution of worm-like micelles and a polymer solution. The simulation parameters of the two model fluids were chosen to match the experimental flow behaviour of these solutions, i.e. the storage and loss moduli and the shear thinning viscosity. Under shear flow, the colloids are observed to align along the flow direction in the worm-like micellar solution, see figures, while the colloids remain randomly distributed in the sheared polymeric fluid and in the quiescent fluids, in excellent agreement with experiments [1]. By analysing the simulation results at the particle level, we obtain a physical explanation of this non-equilibrium ordering

effect. The simulations also explain the shear-induced segregation by size of bidisperse colloids in a worm-like micellar solution [2]. In a polymer solution confined between two moving walls, the suspended colloids are observed to drift to the nearest wall. Simulations of other polymeric systems are under way.



The alignment of colloids (blue) in a worm-like micellar solution (grey) under shear flow. The flow is in the horizontal direction, the flow gradient in the vertical direction.

REFERENCES

[1] I.S. Santos de Oliveira W.K. den Otter and W.J. Briels, *J. Chem. Phys.*, **137**, 204908, 2012.

[2] I.S. Santos de Oliveira, W.K. den Otter and W.J. Briels, *EPL* **101**, 28002, 2013.