P.35 Simulation of the linear and non-linear rheology of viscoelastic polymer solutions

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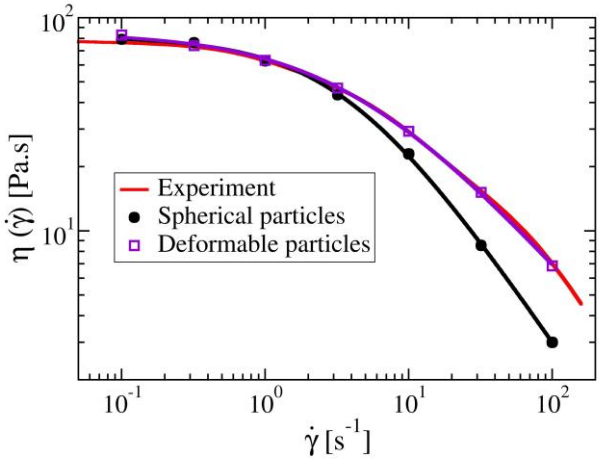
The use of coarse-grained approaches for the simulation of polymer liquids allows access to substantially larger time and length scales that are impossible to reach through atomistic simulations. Coarse graining of any polymer system simplifies both the polymer representation and the description of toplogical constraints or inter---polymer entanglements. Various degrees of coarse-graining are possible such as representing a group of monomers as a blob or bead to a highly coarse-grained view where each entity is described as a point particle.

We present simulation results of the linear and non-linear rheology of two viscoelastic polymer solutions using a highly coarse-grained approach known as the Responsive Particle Dynamics (RaPiD) model. RaPiD, which is a mesoscopic model based upon Brownian dynamics, has been successfully employed for the simulation of shear banding, particle alignment and chain diffusion in viscoelastic fluids [1]. In RaPiD each constituent polymer has until now been viewed as a spherical particle with the effects of the eliminated degrees of freedom included through the selection of an appropriate free energy and transient pair-wise force. Here we update the particle description to account for particle deformability by allowing all RaPiD particles to elongate. The inclusion of this particle deformation is shown to be crucial towards recovering the experimental non-linear rheology i.e. shear thinning effects, for both polymer solutions. We also preserve the description of the linear rheology with the update to the deformable particle representation [2].



Demonstration of the recovery of the non-linear rheology of a polymer solution using the RaPiD deformable particle model.

[1] I.S. Santos de Oliveria, A. van den Noort, J.T. Padding, W.K. den Otter and W.J. Briels, J. Chem. Phys. 135, 104902, (2011)

[2] I.S. Santos de Oliveria, B.W. Fitzgerald, W.K. den Otter and W.J. Briels, *submitted* to J. Chem. Phys