SMOOTHED DISSIPATIVE PARTICLE DYNAMICS MODEL FOR POLYMER SOLUTIONS

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The properties of the dilute and semi-dilute polymer solutions are investigated under simple shear and Poisuelle flow regime by Smoothed Dissipative Particles Dynamics. SDPD is a mesoscopic meshless method with implicit solvent modeling. The method is a thermodynamically consistent version of Smoothed Particle Hydrodynamics (SPH) able to discretize the Navier-Stokes equations and to incorporate thermal fluctuations according to the fluctuation-dissipation theorem. The crucial advantage of the method is applicability to the cases involving complex flow. The microscopic model of the polymer molecule consists of a linear chain composed of several SDPD particles interacting via finitely expendable nonlinear elastic spring.

In the previous work (Phys. Rev. E 77 (2008) 066703-12) we showed that hydrodynamics interactions (HI) are captured for the single polymer. In this work the model is extended to the solutions of the polymers. The dependencies of the static (radius of gyration, structure factor, alignment), dynamic (relaxation time, mean squares displacement), and rheological (shear viscosity, stress coefficients) parameters on the polymer concentration, polymer size is determined. In the simple shear the results are compared with theoretical. scaling predictions (J. Chem. Phys. 133, 164905 (2010)).

For Poisuelle flow dynamic simulations were performed with initially stretched polymers relaxing in the flow. The relationship between microscopic parameters of the polymers and the flow velocity profile is discussed.

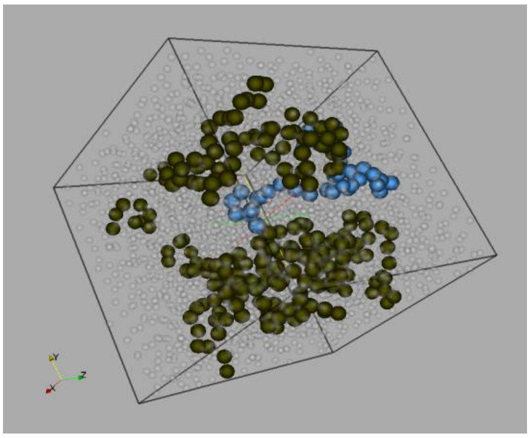

Figure 1: Simulation domain, 6 polymers with 40 beads, one polymer is highlighted (shown in blue), smaller semi-transparent spheres are solvent particles.