MACROMOLECULES IN FLOW FIELDS

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Experimental studies of individual DNA molecules in steady shear flow by fluorescence microscopy have provided a wealth of information on single polymer dynamics [1,2]. In particular, these experiments reveal remarkably large conformational changes due to tumbling motion, i.e., a polymer stretches and recoils in the coarse of time. Since shear flows are omnipresent in biological systems and technical applications, e.g., microfluidics, the understanding of the dynamics of semiflexible polymers – such as DNA – is of great practical interest. The microscopic conformational properties affect the macroscopic rheological behavior of the polymer solution, and hence a detailed theoretical description of the microscopic dynamics is desirable. The dynamic behavior of a macromolecule in shear flow is governed by various parameters; aside from the shear rate, the finite chain extensibility is of major importance.

Employing hybrid mesoscale hydrodynamics simulations, which combine molecular dynamics simulations of the polymer with the multiparticle collision dynamics (MPC) approach for the fluid [3], we studied the non-equilibrium behavior of polymer solutions in shear flow. MPC is a particle-based simulation approach for a fluid, which correctly reproduces hydrodynamic properties and includes thermal fluctuations [3]. By this approach, we find that polymers in both, dilute and semidilute solutions exhibit large deformations and a strong alignment with the flow [4]. More importantly, in the stationary state, the conformational and rheological properties for various concentrations are universal functions of the Weissenberg number with a concentration-dependent relaxation time. Hence, with increasing concentration, hydrodynamic interactions affect the conformational and rheological properties only via the increasing relaxation time. Moreover, dynamical properties – orientational distribution functions and tumbling times – depend on concentration in excess to the relaxation time, a dependence, which we attribute to screening of hydrodynamic interactions in semidilute solution [5].

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