129c Development of Mesoscopic Models for Non-Newtonian Flow Calculations

Patrick T. Underhill and Patrick S. Doyle

The use of mesoscopic or "molecular" models of polymers is becoming more prevalent, both in micro-macro type flow calculations and in comparisons with single molecule experiments. We have examined a new method for generating coarse-grained models of polymers. The resulting models consist of bead-spring chains with the spring force-law taken from the force-extension behavior in the constant extension ensemble. We have applied the method to the freely-jointed chain, including the case of non-equal rod lengths showing the effect of varying flexibility in the chain. The method was also used to generate a bead-spring model of F-actin, which shows how the method is not restricted to one molecular model and can even be applied to experimental data. The current limitations of the method are discussed, including the need for approximate bending potentials to model the worm-like chain with a bead-spring chain. We discuss practical issues such as using the bead-spring models in Brownian dynamics simulations and develop a simple spring force-law that can accurately represent a freely-jointed chain with only a few rods per spring. The development and use of coarse-grained models is also possible for systems that can form more complex architectures.