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Many-Body Dissipative Particle Dynamics Simulations of Polymer Solutions: Hydrodynamic Interactions and Entanglements[1] XIN YONG, Binghamton University — Using many-body dissipative particle dynamics (MDPD), I model polymer solutions with concentrations spanning dilute and semidilute regimes and examine static and dynamic properties of polymer chains, focusing on hydrodynamic interactions and entanglements. The parameterization of MDPD interactions for solvated polymer chains in a liquid-vapor coexistent state is first established by mapping to the mean-field Flory-Huggins theory. The coil-globule transition of polymer chains in dilute solutions is characterized by varying solvent quality and measuring the radius of gyration and end-to-end distance. Both static and dynamic scaling relations for polymer chains in poor, theta, and good solvents are in good agreement with the Zimm theory in which the hydrodynamic interactions are considered. Semidilute solutions with polymer volume fractions up to 0.7 exhibit the screening of excluded volume interactions due to chain overlapping and subsequent shrinking of coils in the good solvent. Furthermore, entanglements become dominant in the semidilute solutions, which inhibit diffusion and relaxation of chains. Quantitative analysis of topology violation confirms that entanglements are correctly captured in the MDPD simulations.

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