DYNAMICS AND RHEOLOGICAL PROPERTIES OF ENTANGLED POLYMERIC SYSTEMS BY DISSIPATIVE PARTICLE DYNAMICS

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Dissipative Particle Dynamics (DPD) is one of coarse-grained level simulation techniques for soft materials that have been applied to a large array of systems such as Newtonian fluids, colloids, polymeric systems and so on. In DPD a conservative force parameter relates to the chemical potential, which, in principle, makes it suitable to study polymer blend, co-polymer and polymer nano-composites. Although many publications show the possibilities of the method, it has some drawbacks such as "bond-crossing" due to soft potentials, which affects to dynamics of polymer chains. Lahmar et al. recently proposed a simulation DPD method coupled with Monte Caro (MC) method that provides Gaussian statistics and 3.2-power law on viscosity, which are reasonable, but shows unphysical properties such as non-Gaussian bond length distribution and no sign of entangled structures in the radius of gyration. In this work we present a modified DPD model that includes entanglement forces. The predictions by this method show 1) Gaussian statistics, 2) Gaussian bond distribution, 3) signs of entanglement effects in radial distribution function, 4) reasonable mean square displacement of entangled polymeric systems, which fits to tube model's prediction, 5) transition of linear viscoelastic properties (the storage modulus G' and loss modules G") from Rouse's behavior to reptation behavior with increasing molecular weight, 6) shear thinning, 7) shear and normal-stress difference stress overshoot upon start-up of shear at high shear rates.