Brownian Dynamics Simulation of Dendrimers and Hyperbranched Polymers under Flow

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Brownian dynamics simulations of perfectly branched dendrimers up to the sixth generation and hyperbranched polymers have been performed under the influence of uniaxial flow. A freely jointed bead−rod model with excluded volume both with and without hydrodynamic interactions has been used. The dependences of conformational properties and the intrinsic elongational viscosity on the flow rate were obtained. The coil−stretch transition was observed for dendrimers of all generations and hyperbranched polymers with it being less pronounced than the same type of transition observed for a linear polymer chain. The transition is observed to occur in two stages as it was for a linear polymer. The dendrimer and hyperbranched polymers first orient at low flow rate as a whole along the flow axis without significant deformation and local orientation. Increasing flow rate leads to local orientation on the level of the monomer leading to significant global deformation. The onset of the coil−stretch transition occurs at lower elongational rates as the number of monomers, N, within the dendrimer and hyperbranched polymers increases. The dependence of the onset of this transition with N is less pronounced than for linear chain, become less steep with N and not described by a power law. Significant influence of degree of branching and Wiener index on behaviour of hyperbranched polymers under flow was shown.