

Flow Behaviour of Associative Telechelic Polymer Melts and Solutions: A Computer Simulation Study

Anoop Varghese, Dipesh Amin and Zuowei Wang

School of Mathematical, Physical and Computational Sciences, University of Reading,
Whiteknights, PO Box 220, Reading RG6 6AX, UK

Nonequilibrium computer simulations have been performed to study the nonlinear rheological and dynamic behaviour of supramolecular polymer networks (SPNs) formed by associative telechelic chains and their non-associative polymer counterparts in both melts and solutions. The startup shear and extensional flow behaviour, as well as the steady-state viscosities, were investigated systematically as functions of the association energy of the sticky end groups, degree of polymerization and flow rate. The steady-state shear viscosities show a general shear-thinning behaviour in the SPN and non-associative polymer melts and solutions, while both the non-associative and associative polymer melt systems demonstrate extensional thickening behaviour in steady state for chain lengths ranging from unentangled to weakly entangled regime. The observed nonlinear behaviour can be well interpreted using the flow-induced non-Gaussian chain stretching, chain segment reorientation, and reduction in the probabilities of sticky group association.