

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Segmental orientation dynamics in bidisperse entangled linear polymer melts ZUOWEI WANG, JING CAO, ALEXEI LIKHTMAN, Department of Mathematics and Statistics, University of Reading, Whiteknights, RG6 6AX, UK, RONALD LARSON, Department of Chemical Engineering, University of Michigan, Ann Arbor, MI 48109-2136 — Extensive molecular dynamics simulations were performed to investigate the segmental orientation dynamics in mono- and bidisperse entangled linear polymer melts. The binary blends consist of short probe chains diluted in long chain matrices of chain length up to 30 entanglements. With increase of the chain length in monodisperse melts, the bond vector autocorrelation function was found to approach a distinctive time-dependent power law, which is compared with recent NMR experiments. When introduced into long chain matrices, the segmental orientation relaxation and monomer diffusion of short probe chains slowed down strongly due to the suppression of constraint release (CR) effects. The same trend was observed for the end-to-end vector correlation function, reflecting the CR effects on contour length fluctuations. On the other hand, the time-dependent orientation coupling parameter in the entangled systems demonstrates the similar universal behaviour as that discovered in unentangled melts. Considering the stress-optical law was recovered in all simulated systems, our simulations should clarify the connection between rheology and other experimental techniques, which are essential for progress in modeling entangled polymers.

Zuowei Wang
Department of Mathematics and Statistics,
University of Reading, Whiteknights, RG6 6AX, UK

Date submitted: 27 Nov 2010

Electronic form version 1.4