Multiscale simulations of chain dynamics in polymeric liquids undergoing shear BAMIN KHOMAMI, JUN KIM, BRIAN EDWARDS, University of Tennessee, MATERIALS RESEARCH AND INNOVATION LABORATORY TEAM — Multiscale simulations were performed of a polyethylene liquid at the atomistic, mesoscopic, and continuum levels of description. Molecular dynamics of shear flow at the atomistic level provided a fundamental description of the rheological properties and the dynamical information concerning individual chains. At low shear rates, the dynamics are dominated by the chain-stretching mode, whereas correlations of the chain end-to-end vectors indicated distinct tumbling frequencies at high shear rates. A mesoscopic model was developed based on the concept of a bead-spring chain in a mean field representing the surrounding chains using an anisotropic diffusion matrix. Brownian dynamics simulations revealed quantitative agreement between these two models for the rheological properties, the tumbling frequencies of the individual chains, and the extensions of the chains. The mesoscopic model was reduced to a continuum model by averaging the bead-spring chain model. This model predicted the simulation data quantitatively at low shear rates, but greatly over-predicted the data at high shear rates where the tumbling dynamics of the individual chains dominated the system response.

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