

Abstract Submitted
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Multi-level slip-link modeling JAY SCHIEBER, Illinois Inst of Tech

— That the dynamics of concentrated, high-molecular-weight polymers are largely governed by entanglements is now widely accepted, and typically understood by the tube model. Although the original idea for slip-links was proposed at the same time as tubes, only recently have detailed, quantitative mathematical models arisen based on this picture. We argue here for the use of a slip-link model that has strong connections to atomistic, multichain levels of description, agrees with non-equilibrium thermodynamics, applies to any chain architecture and can be used in linear or non-linear rheology. We present a hierarchy of slip-link models that are connected to each other through successive coarse graining. One might choose a particular member of the hierarchy depending on the problem at hand, in order to minimize computational effort. In particular, the most detailed level of description has four parameters, three of which can be determined directly from atomistic simulations. The least-detailed member is suitable for predicting non-linear, non-uniform flow fields. We will show how using this hierarchy of slip-link models we can make predictions about the non-linear rheology of monodisperse homopolymer melts, polydisperse melts, or blends of different architectures.

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