Unveiling Polymer Viscoelasticity Through Bead-Rod Modeling

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Abstract

One good way to explain the elasticity of a polymeric liquid is to consider the orientation distribution of the macromolecules. When exploring how macromolecular architecture affects the elasticity of a polymeric liquid, we find general rigid bead-rod theory to be both versatile and accurate. This theory sculpts macromolecules using beads and rods: beads represent points of Stokes flow resistance, while rods represent rigid separations. In this way, the influence of macromolecular shape on its rheological behavior in suspension is determined. Our work highlights recent advances in polymer viscoelasticity using general rigid bead-rod theory, including the discovery of the first new materials functions from this framework since the complex viscosity of Hassager (1974). These include steady shear material functions [1], large-amplitude oscillatory shear flow material functions [2], and steady uniaxial [3], biaxial [3], and planar extensional viscosities [4]. Additionally, recent studies have expanded upon oscillatory superposition on steady shear flow, with significant developments in both parallel and orthogonal superposition [5,6]. In particular, the latest advancements in parallel superposition have provided deeper insight into the nonlinear viscoelastic response of polymer solutions, revealing intricate dependencies on molecular architecture and flow history. We find that each of these material functions depends upon the same molecular feature: the ratio of the macromolecular moment of inertia about the molecular axis to that about the axes transverse to the molecular axis. We then use these new material functions to bridge the Oldroyd 8-constant framework (and thus all of its many special cases) to general bead-rod theory [7], further solidifying its role in predicting polymer rheology across diverse flow conditions.

Keywords: general rigid bead-rod model; complex viscosity; viscoelasticity; orientation, extensional viscosity parallel superposition.

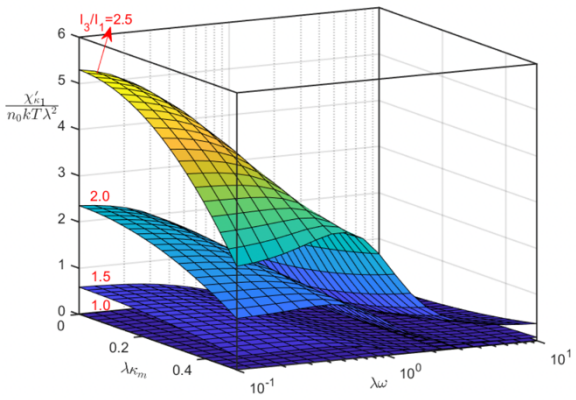

Figure 1. Dimensionless normal stress coefficient as a function of dimensionless frequency and dimensionless mean shear rate for oblate macromolecules. The curves correspond to different ratios of the first to second normal stress differences, with values indicated in red.