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Tumbling dynamics of isolated polymer chains in strong shear flows and the effects of chain resolution RONALD LARSON, INDRANIL SAHA DALAL, ALEX ALBAUGH, University of Michigan, NAZISH HODA, ExxonMobil Upstream Research — Using Brownian dynamics simulations, without hydrodynamic and excluded volume interactions, on polymer chain models encompassing a wide range of resolutions, we present a detailed investigation on the behavior of isolated chains in shear flow. We find a highly non-monotonic behavior for all models, with chain compression occurring at ultra-high shear rates that is consistent with the recent simulation studies. However, results obtained using highly refined models, with resolutions lower than a Kuhn step, reveal that this transition is an artifact of the level of chain discretization. Also, our results clearly indicate that, at high shear rates, the chain thickness in the shear-gradient direction is independent of the chain length, which differ from previously reported scaling law. We show that the chain thickness is fixed by the distance a sub-section of the chain can diffuse in the shear-gradient direction before convection stretches it out and suppresses further diffusion. Simple physical arguments are then used to derive the correct scaling laws for the coil width and the tumbling time at high shear rates. We believe that our findings presented here will provide the foundation for a better understanding of this basic problem in polymer dynamics.

Ronald Larson
University of Michigan

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