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Brownian dynamics of wall tethered polymers in shear flow[1]

TIRAS Y. LIN, AMIR SAADAT, AMIT KUSHWAHA, ERIC S.G. SHAQFEH, Stanford University — The dynamics of a wall tethered polymer in shear flow is studied using Brownian dynamics. Simulations are performed with bead-spring chains, and the effect of hydrodynamic interactions (HI) is incorporated through Blake's tensor with a finite size bead correction. We characterize the configuration of the polymer as a function of the Weissenberg number by investigating the regions the polymer explores in both the flow-gradient and flow-vorticity planes. The fractional extension in the flow direction, the width in the vorticity direction, and the thickness in the gradient direction are reported as well, and these quantities are found to compare favorably with the experimental data of the literature. The cyclic motion of the polymer is demonstrated through analysis of the mean velocity field of the end bead. We characterize the collision process of each bead with the wall as a Poisson process and extract an average wall collision rate, which in general varies along the backbone of the chain. The inclusion of HI with the wall for a tethered polymer is found to reduce the average wall collision rate. We anticipate that results from this work will be directly applicable to, e.g., the design of polymer brushes or the use of DNA for making nanowires in molecular electronics.

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