224e Using Bead-Spring Repulsions to Model Entanglement Interactions in Brownian Dynamics of Bead-Spring Chains

Sean P. Holleran and Ronald G. Larson

We have developed a bead-spring Brownian dynamics simulation method for modeling the interaction between electrophoretically translating DNA strands and an immovable post. The use of a bead-spring approach will allow for the simulation of polymer chains too long to be simulated by bead-rod techniques. Our new method determines the shortest distance between individual springs and the post, calculates a repulsive force inversely related to the distance using an exponential form, and corrects for the rare situation when a spring passes beyond the post. We consider hairpin collisions with a single post in weak electric fields. We use the x-displacement, the spatial separation between a chain that collides with the post and an unhindered molecule translating at the free velocity, as a measure of the influence of the post on chain mobility, and to compare with previous simulations performed using a bead-rod method (Shaqfeh and Patel, 2003). Previously published results show that x-displacement is unchanged by increasing velocity in the limit of high Peclet number ($Pe > 1.0$). We find that x-displacement linearly increases with increasing velocity in the limit of low Peclet number ($Pe < 0.1$), and that our low Peclet results are consistent with those for the bead-rod model at $Pe > 1.0$. Our new method is a general one that allows us to compute the effects of entanglements in systems with rare entanglements and long chains that cannot be simulated by any other method.