485c Time Scales in Polymer Electrophoresis through Narrow Constrictions: a Brownian Dynamics Study

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Brownian dynamics simulations are used to characterize the time scales involved in polymer electrophoresis through narrow constrictions. The polymer is modeled as a freely jointed bead-rod chain with a total charge distributed uniformly among the beads. The narrow constriction is a channel with a thin region of height $h_s < R_g$ which separates two thicker regions, both of height $h_l \sim R_g$, where R_g is the polymer radius of gyration. The polymer is initially placed in a thick region, and an applied electric field drives it into the next thick region through the intervening narrow constriction. The polymer electrophoresis is characterized by three time scales, each of which depends on the polymer chain length, N. An approach time, t_{app}, describes the motion of the polymer to the entrance of the thin region. Upon reaching the entrance of the thin region, the polymer is entropically trapped and its escape from the trap is associated with an activation time, t_{act}. After the activation event, the motion of the polymer through the thin region and into the next thick region is characterized by a crossing time, t_{cross}. Whereas t_{app} and t_{act} decrease with increasing N, t_{cross} increases with increasing N. As a consequence, the transit velocity of the polymer, $v_{transit}$, first increases with increasing N, and then decreases beyond a certain value of N. The position of the maximum in $v_{transit}$ is shown to depend on the applied electric field strength, the relative values of h_s and h_l, and whether channel is two dimensional or three dimensional. We discuss the relevance of this behavior to transport of polymers in microfluidic channels exhibiting entropic trapping effects and to translocation of polymers through nanopores.