485a Brownian Dynamic Simulations of Electrophoresis and Electro-Stretching of DNA Molecules

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We derive a model for the motion of long DNA chains entangled in a concentrated gel matrix in the presence of a strong electric field. The model is adapted from a tube-based slip-link approach, which was originally intended to model the rheology of entangled polymer fluids, and is suitable for solution by Brownian dynamic simulation. We account for: the constraining effect of the surrounding matrix, motion due to the electric field and finite extensibility of the DNA chain. We are able investigate the effect of molecular weight and field strength on the DNA drift velocity in a constant electric field, along with molecular stretching in an oscillating field. Both examples have applications in DNA separation and sequencing. Our approach includes a detailed treatment of the chain end motion through the matrix, which our simulations demonstrate has a significant role in the DNA dynamics, particularly in oscillating fields. The model provides a convenient formalism for further refinements. For example, large fields may tend to cause hernia-like chain loops to protrude from the main tube. Furthermore, to model matrices comprised of linear polymers we can include the effect of constraint release, in which the confinement experienced by the DNA is diminished by the motion of the matrix chains.