Mesoscopic Simulations of Electroosmotic Flow and Electrophoresis in Nanochannels

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We present dissipative particle (DPD) simulations of electrolyte flow in nanochannels for varying salt concentration and surface slip conditions. First, a method is presented by which the slip length $\delta_B$ at the channel boundaries can be tuned systematically from negative to infinity by introducing suitable wall-fluid friction forces. Using this method, we study electroosmotic flow (EOF) in nanochannels in different electrostatic regimes for varying surface slip conditions. The results are compared with corresponding simulations using coupled Lattice-Boltzmann/Molecular Dynamics (LB/MD). For the weak-coupling regime, analytic expressions for the flow profiles in the presence of partial-slip as well as no-slip boundary conditions are derived from the Poisson-Boltzmann and Stokes equations, which are in good agreement with the numerical results. Finally, we investigate the influence of EOF on the effective mobility of polyelectrolytes in a nanochannel. Analytic expressions for the electroosmotic mobility and the total mobility are derived which are in good agreement with the numerical results. The relevant quantity characterizing the effect of slippage is found to be the dimensionless quantity $\kappa \delta_B$, where $1/\kappa$ is an effective electrostatic screening length at the channel boundaries.