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Effects of Relaxation on Drag Force and Diffusivity of Highly Charged Spherical Particles in Cylindrical Pores

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Diffusion of macromolecules through nanopores of comparable sizes is affected by an interaction between the particle and the confining entities including both hydrodynamic and electrostatic interactions. The particle-pore hydrodynamic interaction causes an increase in the drag force exerted on the particle, resulting in the reduction of its diffusivity. If the particle is charged and submerged in an electrolytic solution, the particle motion creates a distortion of the electrical double layer, resulting in an excess retarding force added to the usual enhanced hydrodynamic drag. This is commonly known as the relaxation effect. In the present work, the excess force due to relaxation was evaluated from the finite element solution of the governing equations including Stokes equation, Poisson's equation and Nernst-Planck equations. The regular perturbation scheme involving the Peclet number was employed, considering the particle translocation as a perturbation on equilibrium state. The enhanced drag due to relaxation and the particle diffusivity are obtained for spherical particles confined in cylindrical pores where the particle and pore wall are of like charge and the electric potential of the system is high enough that the Poisson-Boltzmann could not be linearized. The obtained results are compared to effects of relaxation on drag force and diffusivity of macromolecules calculated by employing the perturbation involving the dimensionless surface charge density.

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