221c Brownian Dynamics Simulations of Shear-Induced Migration of DNA Molecules in Dilute Solutions near a Solid Boundary

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Recent experiments show that DNA molecules migrate away from solid boundaries in shear flow, and a depletion layer is formed at the steady state. In channel flows, Jendrejack et al. [J. Chem. Phys., 119, 1165 (2003)] have modeled this phenomenon using Brownian dynamics (BD) simulations of a bead-spring model with full hydrodynamic interaction (HI), where a finite element method was used to obtain the hydrodynamic tensor including the wall effect. While this method is successful, the hydrodynamic tensor must be re-computed for different channel geometry. Here, we propose a modified Rotne-Prager-Yamakawa hydrodynamic interaction tensor to describe the hydrodynamic interaction between two spheres with a wall nearby. This newly developed tensor is suitable for Brownian dynamics simulations because it accounts for both the finite volume of the beads and the effect of the presence of a stationary boundary. The tensor obeys the reciprocity relation that originates from self-adjointness of the Stokes operator, and therefore the ad hoc average used to enforce this reciprocity relation in earlier approximations can be avoided. As an initial step, BD simulations of a dumbbell showed that our method yields results similar to those obtained from a kinetic theory for dumbbells near a wall in the presence of shear [Jendrejack et al., J. Chem. Phys., 120, 2513 (2004)]. Finally, We carry out Brownian dynamics simulations with multiple beads and compare the predictions with the experimental configurations and concentrations of DNA molecules in shear flow near a surface reported by Fang et al. [J. Rheology, 49, 127(2005)].