

Hydrodynamic Interactions of Polyelectrolyte Complex Fluids in Microchannels Confined Between Planar Walls

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Hydrodynamic interactions (HI) play an essential role in the dynamics of polyelectrolyte chains confined in micro/nanochannel environments. In this study, we propose a new computational method to describe the HI of polyelectrolytes confined between two parallel plates in the context of Brownian dynamics (BD) simulations. The method is based on the Green's function for the flow field generated by a point force in the channel. The far-field effect, dominant when the bead-bead and bead-wall separations are large compared to the bead hydrodynamic radius, can be well described with this point force approximation. The mobility of a single sphere modified by the walls is also derived from the Green's function. A further improvement to include the finite size effect of the beads is faithfully explored. The feasibility of the method is demonstrated by BD simulations of the diffusion of confined bead-spring chains. (This work was supported by the Basic Research Funds R01-2004-000-10944-0 from the KOSEF.)