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Modeling of mesoscopic electrokinetic phenomena using charged dissipative particle dynamics[1] MINGGE DENG, ZHEN LI, GEORGE KARNIADAKIS, Brown University — In this work, we propose a charged dissipative particle dynamics (cDPD) model for investigation of mesoscopic electrokinetic phenomena. In particular, this particle-based method was designed to simulate micro- or nano- flows which governing by Poisson-Nernst-Planck (PNP) equation coupled with Navier-Stokes (NS) equation. For cDPD simulations of wall-bounded fluid systems, a methodology for imposing correct Dirichlet and Neumann boundary conditions for both PNP and NS equations is developed. To validate the present cDPD model and the corresponding boundary method, we perform cDPD simulations of electrostatic double layer (EDL) in the vicinity of a charged wall, and the results show good agreement with the mean-field theoretical solutions. The capacity density of a parallel plate capacitor in salt solution is also investigated with different salt concentration. Moreover, we utilize the proposed methodology to study the electroosmotic and electroosmotic/pressure-driven flow in a micro-channel. In the last, we simulate the dilute polyelectrolyte solution both in bulk and micro-channel, which show the flexibility and capability of this method in studying complex fluids.

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