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Accurate treatment of external electric field in molecular dynamics simulation of nanofluidics ANJAN RAGHUNATHAN, NARAYANA ALURU, Beckman Institute of Advanced Science and Technology, University of Illinois at Urbana-champaign, Urbana, IL 61801 — We propose a self-consistent molecular dynamics (SCMD) formulation for electric-field-mediated transport of water and ions through a nanochannel connected to reservoirs. The SCMD formulation is compared with a uniform field MD approach, where the applied electric field is assumed to be uniform, for 2 nm and 3.5 nm wide nanochannels immersed in a 0.5M KCl solution. The reservoir ionic concentrations are maintained using the dual-control-volume grand canonical molecular dynamics technique. Simulation results with varying channel height indicate that the SCMD approach calculates the electrostatic potential in the simulation domain more accurately compared to the uniform field approach, with the deviation in the results increasing with the channel height. The translocation times and ionic fluxes predicted by uniform field MD can be substantially different from those predicted by the SCMD approach. Our results also indicate that during a 2 ns simulation time K^+ ions can permeate through a 1 nm channel when the applied electric field is computed self-consistently, while the permeation is not observed when the electric field is assumed to be uniform.

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