

Abstract Submitted
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Field-Biased Molecular Simulation Technique for Polyelectrolytes

AMIR VAHID, Chem Eng Dept The University of Akron Akron OH 44325-3906, J. RICHARD ELLIOTT — External fields can be used to impose density profiles in inhomogeneous fluids and interfacial phenomena¹. In this study an electric field has been imposed on 1372 hard spheres through 20 negative point charges and 20 positive charges. Also, the effect of partial charges was investigated on a polyelectrolyte with implicit and explicit solvent. Long-range interactions are considered through particle-mesh Ewald summation and its pairwise alternatives. It has been found that it is not necessary to update the Coulombic interactions after each time-step. Energy is conserved even after many numbers of time-steps. Therefore, the computation time for the long-range interaction is less than the discontinuous molecular dynamic (DMD) and/or discontinuous Monte Carlo components. This means that the forced-biased discontinuous molecular simulation method is viable for future studies of confined fluids containing interface and ionic liquids as performed with a field-biased conventional molecular dynamic method by Wardle et al. Finally, the effect of the biased method on dihedral angle is investigated.

Amir Vahid
Chem Eng Dept The University of Akron Akron OH 44325-3906

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