

A Novel Monte Carlo Algorithm for Simulating Strongly Associating Fluids: Applications to Water, Hydrogen Fluoride, and Acetic Acid

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Abstract

A novel aggregation-volume-bias Monte Carlo (AVBMC) algorithm is presented which greatly enhances the efficiency of sampling the phase space of fluid systems consisting of strongly associating molecules. The algorithm is compared to the bond-bias Monte Carlo (BBMC) algorithm by Tsangaris and de Pablo [*J. Chem. Phys.* **101**, 1477 (1994)] and the monomer-addition-subtraction algorithm (MASA) algorithm by Visco and Kofke [*J. Chem. Phys.* **110**, 5493 (1999)]. The AVBMC algorithm is easy to implement, generally applicable, and robust. The efficiency of the AVBMC algorithm is demonstrated for a large variety of processes and systems, including the vaporization of a liquid methane droplet or of a water cluster, an investigation of the temperature- and pressure dependent properties of superheated hydrogen fluoride vapor, and the vapor-liquid coexistence curve of acetic acid.

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