The Calculation of Chemical Potential of Organic Solutes in Dense Liquid Phases by Using Expanded Ensemble Monte Carlo Simulations

장재언*
서울시립대학교 화학공학과
(changjaee@uos.ac.kr*)

The chemical potentials of organic compounds in dense liquid phases are calculated by using expanded ensemble Monte Carlo simulations. To make insertion of a solute molecule efficiently, Lennard-Jones size parameters and bond lengths are varied with coupling parameter. A robust adaptive scheme is proposed in order to determine biasing weights during the simulation. Using the proposed simulation technique, chemical potentials of organic molecules in dense liquid phases are obtained from a single run of simulation. The excess chemical potentials of several hydrocarbon molecules including n-alkanes, benzene, toluene and ethanol in aqueous phases at infinite dilution as well as in their pure liquid phases are calculated at 298 K and 1 atm, and simulation results for mixtures are compared with experimental data of Henry's constant. Also, a prototype of molecular simulator based on Windows® platform is introduced. The simulator is equipped with graphical user interface, 3-dimensional visualization of molecular system, chart monitoring of simulated properties, easy-to-use model builder and force field setup tool.