

## Derivation of an OPLS-like Force Field for Calculation of VLE for Hydrofluorocarbons from Monte Carlo Simulations

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Monte Carlo (MC) simulations are used in various fields of physical chemistry. Recent advances in computer hardware and algorithmic implementations of MC sampling techniques bring these methods closer to becoming a mainstream tool for prediction and extrapolation of thermophysical data. However, application of MC simulations to the calculation of thermophysical properties normally requires significant computational resources as well as substantial human expertise. In this work we will consider a possibility of decreasing of the expert participation in the calculations by introducing a formal algorithm for determination of the force field parameters. The algorithm represents a bootstrap procedure and includes a step-by-step calculation of the Lennard-Jones well depth and radius for various atomic types. The algorithm was used for optimization of the van der Waals parameters of the OPLS-like force field for hydrofluorocarbons. For each atomic type, liquid densities, saturated vapor pressures, and enthalpies of vaporization at four different temperatures for at least two compounds were used in optimization of the parameters. To determine the response surfaces, twenty five two-box Gibbs ensemble simulations were made at each temperature. The parameters for these simulations were selected according to a central composite design scheme. The obtained force field was then applied to calculation of VLE for hydrofluoroolefin-based refrigerants.