

455h Force Field Parameterization and Calculation of Phase Equilibria for Organic Nitro Compounds

David Rigby and Rajesh Khare

Compounds containing the organic nitro group can be modeled using a number of so-called all atom force fields developed originally for modeling biological or synthetic polymeric materials. However the focus of these force fields is generally on properties of materials at ambient temperatures far removed from the critical temperature, and consequently the performance of such force fields when used directly in calculations of vapor-liquid coexistence curves is largely unknown. In addition, such all atom force fields tend to be rather inefficient for calculations of phase equilibria using techniques such as Gibbs ensemble Monte Carlo simulation in view of the extensive computational requirement from a combination of the large number of atoms needed in all-atom simulations and the long runs required in this type of simulation. As a consequence therefore it is generally desirable to work with united atom force fields when performing such calculations.

In the present work we describe a novel approach to the rapid development of united atom force field parameters using an initial series of simulations performed using an all atom force field. Specifically, we have used the COMPASS all atom force field as a basis for generating parameters for the united atom NERD force field, which is then applied to phase equilibrium simulations. The advantage of this approach is that accurate values of the necessary valence terms have already been obtained within COMPASS using high level ab initio calculations, which allows for rapid determination of the corresponding parameters for use within NERD. The systems chosen to develop the parameterization procedure consist of a series of nitroalkanes. The presentation will discuss issues arising from the lack of a precise mapping of terms between the two force fields (i.e. aspects of the coarse graining problem) in addition to presenting new data for vapor-liquid phase equilibria of compounds capable of being modeled using the NERD force field.