Concentration-dependent charge scaling as a simple method of force field correction in MD simulation of aqueous alcohol solutions

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In molecular dynamics investigations, the choice of the force field is the general problem. Modern force fields are good enough to reproduce the physical properties of a wide range of substances with a rather high accuracy. However, that accuracy is not enough for structure investigations especially in working with mixtures. In this case, either more resource-intensive methods or force field correction are required.

Alcohol-water solutions are an example of such a case where using standard force fields gives insufficient accuracy to predict properties. The polarity of such solutions is known to change dramatically with concentration increase. In standard MD simulations, however, all molecular parameters including atomic charges have to be fixed. We suggest a simple method of force field correction to eliminate this problem – concentration-dependent charge scaling with linear concentration variation of scaling factor. To simplify the method further we scale charges for alcohol molecules only. We have shown that even our simplest form of force field correction allows us to obtain models with much higher accuracy of properties predictions than using standard force fields. The method was constructed to reproduce the concentration behavior of density, but it was shown to reproduce the fine volumetric characteristics like alcohol partial molar volume as well as other characteristics like dielectric permittivity, excess enthalpy, and even chemical potentials.

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