

A Transferable Force Field to Predict Phase Equilibria and Thermodynamic Properties of Carboxylic Acids and Furans

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In order to achieve its sustainable development claims, the chemical industry focuses its R&D activities on new technologies for the modelling and prediction of the physico-chemical behaviour of molecules. These technologies are now integrated in the design stage of chemical products and are involved in all the activities of the chemical industry including the design and optimization of manufacturing processes. In this context, molecular simulation appears as a reliable alternative route to experiments. Indeed, molecular simulation allows predicting the phase equilibrium and the phase properties of pure compounds and mixtures by performing statistical calculations or by solving the equations of classical mechanics for a set of particles interacting via an intermolecular potential fitted on available experimental data. Thus, it is possible to avoid making expensive experiments and to explore thermodynamic conditions that might be unfeasible due to current limitations of experimental devices. In this work we propose a new transferable force field to simulate with the Monte Carlo method phase equilibria and thermodynamic properties of systems involving carboxylic acids and furan-derived compounds. For both molecular families, we have used the Lennard-Jones parameters obtained for the AUA4 force field in previous works for alcohols, ketones and ethers and only the charges on the functional groups have been modified to match the saturation properties of pure compounds. The new force field appears transferable for a wide variety of properties and allows reproducing the structure of the liquid phase as well. Furthermore, binary mixtures have been simulated without introducing any empirical binary interaction parameter.