

PHASE EQUILIBRIA PREDICTION BY MOLECULAR SIMULATIONS: COMPARISON OF DIFFERENT METHODS

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Modern industry faces the challenge of designing, and hence producing, molecules (or molecular ensembles) having well defined chemico-physical characteristics (such as pharmaceuticals, polymers and additives) by fast and economical processes. The recent progress in computer architecture and molecular simulation software have transformed the theoretical models from topics of exquisite academic interest into practical tools for molecular and process design, and thus of industrial relevance. Notwithstanding the progressively increasing importance of molecular simulation in several industrial sectors, still very few papers can be found in the current literature documenting the potential of such applications in chemical engineering.

In this work, we present the results of the prediction of VLE behavior for an extensive set of organic and water systems obtained from molecular simulations based on accurate scaled *ab initio* force fields. The force fields were obtained by scaling the results of *ab initio* calculations performed with the density functional method BLYP and the DNP basis set within the DMol³ package. The scaling procedure uses three parameters and compares the calculated frequencies, infrared and Raman intensities with those obtained by the experimental spectra. We also report, for comparison, the results obtained with a different approach, based on the application of a dielectric continuum solvation model.