

## Molecular Simulation Methods for Prediction of Phase Equilibrium Properties

A.Z. Panagiotopoulos<sup>C, S</sup> and P.J. Lenart

*Department of Chemical Engineering, Princeton University, Princeton, NJ, U.S.A.*

Molecular simulations can now be used routinely for predictions of phase equilibrium properties of industrial important fluids and their mixtures. For vapor-liquid coexistence properties, Gibbs ensemble and Grand-Canonical Monte Carlo simulations with histogram reweighting are commonly used methods [1]. Recently, direct techniques for simulations of equilibria involving solids have also been developed [2]. The main barrier to widespread application of such methods in the chemical industry is the lack of accurate intermolecular potentials (force fields). Potential development methods that use ab initio calculations show significant promise in this regard [3]. Most current force fields do not incorporate non-additive effects (e.g. polarizability) because of the high computational cost. In this presentation, we will review the computational methodologies and summarize the areas of success (and failure) of presently available models. Ongoing research in our group aims to develop models that accurately represent phase coexistence properties over broad ranges of temperatures and densities will be summarized.

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