

Title: Vapor-liquid equilibrium phase diagrams for environmental applications

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Activity coefficients are often predicted by models, like UNIFAC and UNIQUAC. UNIFAC, a group contribution method, is often inadequate for predicting behavior. The parameters needed in the UNIQUAC equation, molecule-molecule interactions, are difficult to measure experimentally but can be determined through computations. For the first time, *ab initio* and molecular mechanics calculations, in combination have been used to successfully calculate interaction parameters to create vapor-liquid equilibrium phase diagrams, that match experimental data, for binary systems of all polarity combinations. Three systems have been used for verification: water and methanol, carbon tetrachloride and acetonitrile, and methylcyclopentane and benzene.

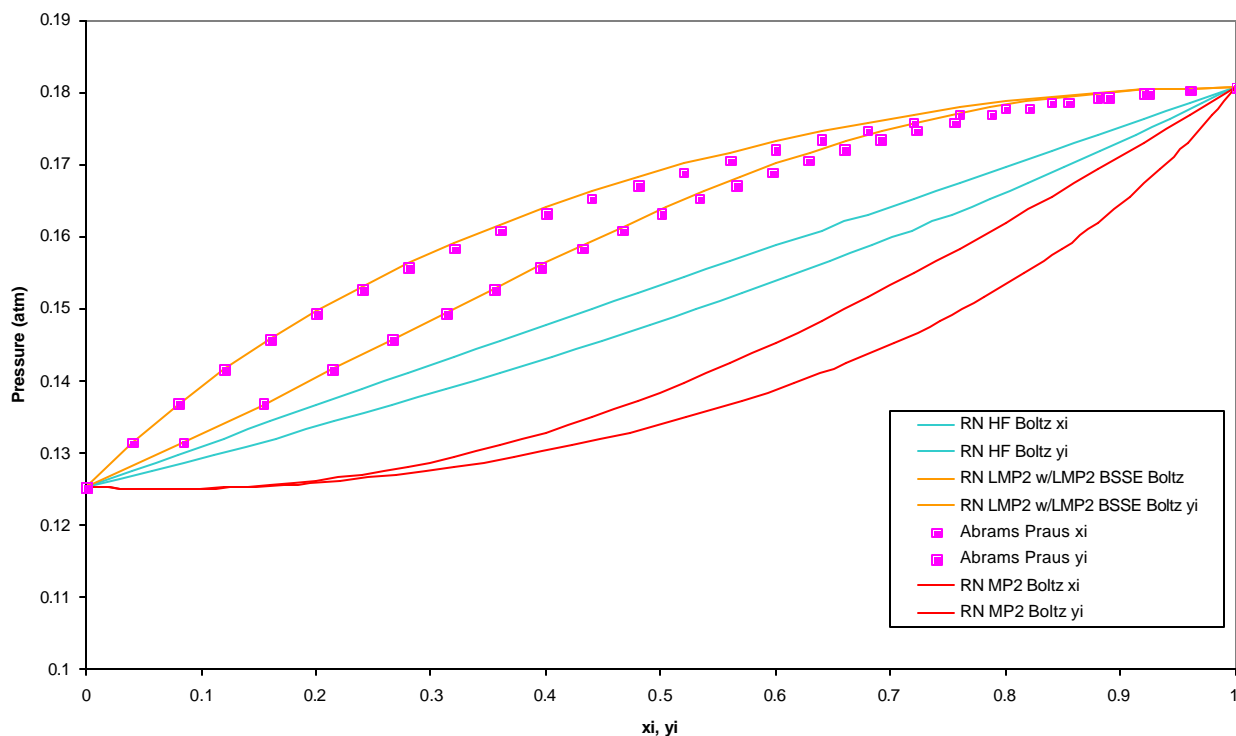


Figure 1. The Boltzmann weighted interaction parameters from the LMP2 method were appropriate for predicting the vapor-liquid equilibrium behavior of MCP and benzene.

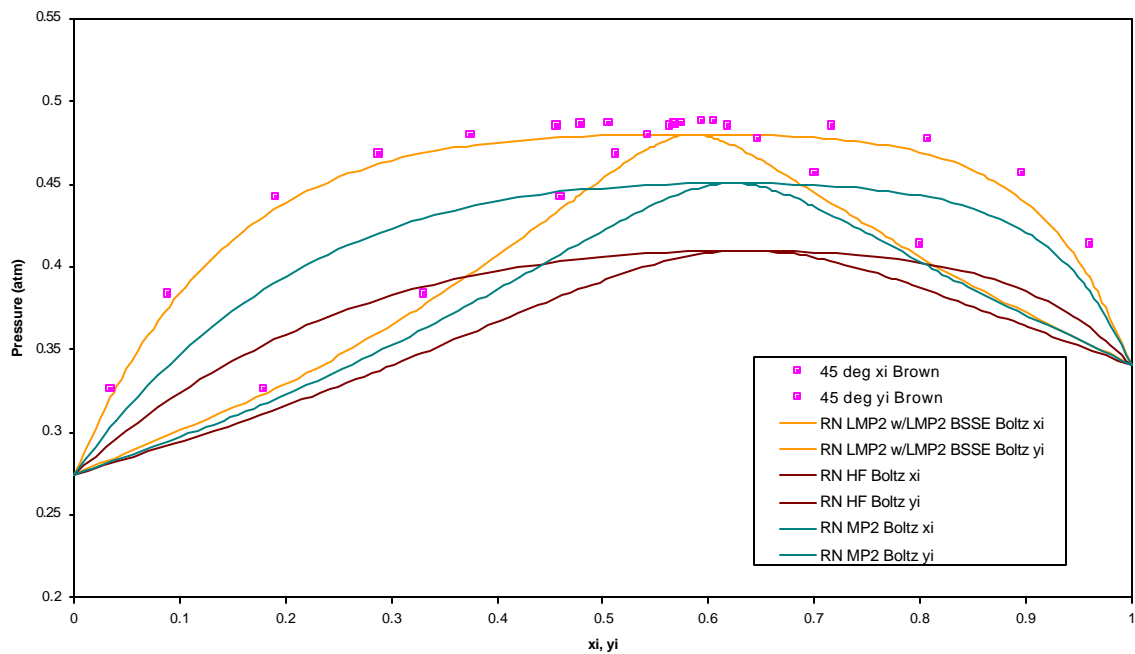


Figure 2. Vapor-liquid equilibrium phase diagram of carbon tetrachloride and acetonitrile. The pink dots are from experimental data. The lines are from different *ab initio* methods for calculating the interaction parameters for the UNIQUAC equation. All of the interaction energies are Boltzmann

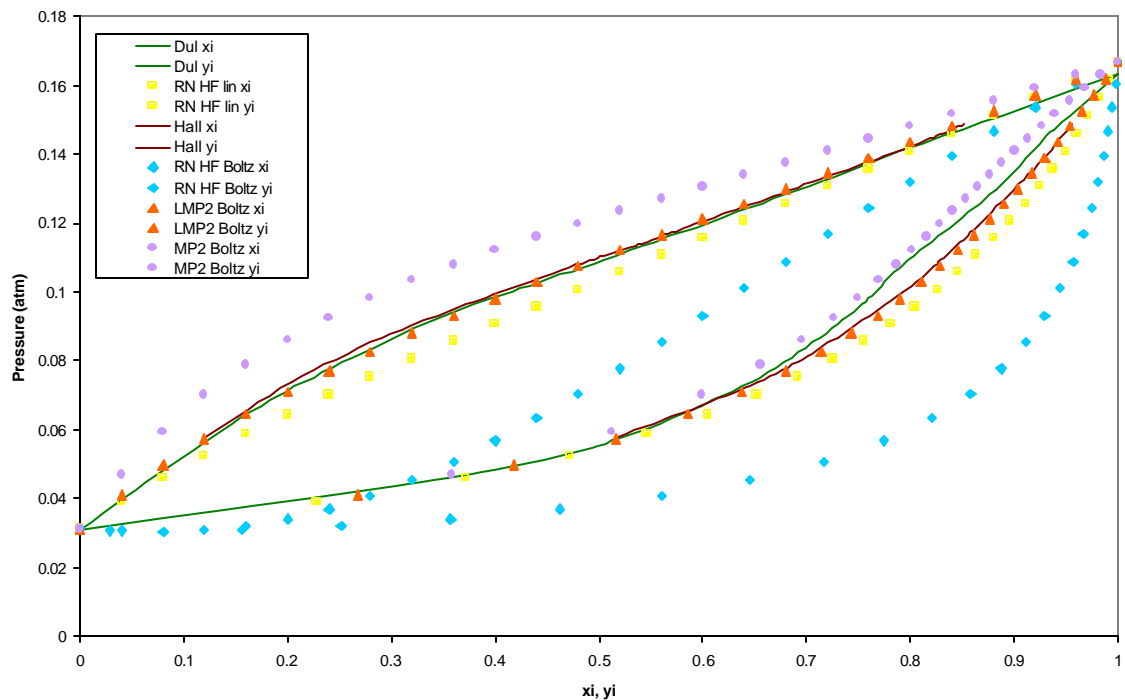


Figure 3. The experimental phase diagrams (solid lines) are compared to the phase diagrams predicted by our method (symbols) for methanol and water. The LMP2 method provides the best

