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Computer Simulations of Vapor-Liquid-Liquid Equilibria Involving Hydrocarbons and Water

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In this work three-phase equilibria between hydrocarbons and water and their mixed vapor phase are studied using Gibbs Ensemble Monte Carlo simulations. In earlier investigations phase equilibria between a single liquid and a single vapour phase of the pure components like water [1], pure hydrocarbons and hydrocarbon mixtures [2] have been the subject of our studies. Optimal parameter combinations for the binary hydrocarbon-water systems were determined earlier [3] and those parameter sets were used in subsequent studies of the two-phase system of liquid water/liquid hydrocarbons [4]. In the present study, the latter system is extended to include a vapor phase in order to more realistically model these systems.

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