

Abstract Submitted
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Testing Theory Against Experiment and Simulation for Chain Fluids: Can Lattice Compete with Continuum?¹ RONALD WHITE, JANE LIPSON, Dartmouth College — We present new results from an in-depth four-way comparison which contrasts the performance of analogous lattice and continuum integral equation theories, with both being held accountable to recently obtained Monte Carlo simulation results and real experimental data. The success of the modeling methods is compared in terms of both experimentally accessible physical properties (e.g., PVT surfaces and coexistence boundaries), as well as the more fundamental underlying quantities, such as free energies, and model internal energies. Without fitting to any mixture data, we find good to excellent predictive ability for mixing behavior, even for the simplest lattice-based approach. Our results lead us to propose the most crucial elements required in constructing simple, yet effective, theories.

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Ronald White
Dartmouth College

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