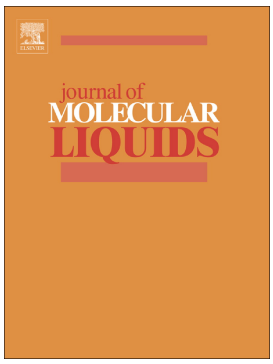

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A review of molecular simulation applied in vapor-liquid equilibria (VLE) estimation of thermodynamic cycles

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Abstract

Thermodynamic cycles such as the organic Rankine cycle (ORC), heat pump cycles and refrigeration cycles are flourishing in both industrial and domestic fields. As a carrier of energy conversion among these cycles, working fluids are considered to be a critical factor affecting the thermal performance. Therefore, studies on their thermophysical properties, particularly VLE, attract increasingly attentions of researchers. However, in terms of researches on some mixed working fluids and new working fluids, some conventional methods are limited because of the lack of experimental data. To solve the dilemma, the molecular simulation (MS) was developed and gradually became an efficient and powerful tool for thermodynamic cycles' analyses. In the present work, a comprehensive review on applications of MS for thermodynamic cycles is presented, and analyses focus on VLE of working fluids. The review first covers the state of the art of MS, including a brief introduction of theoretical