Phase Equilibria and Critical Points of Pentaerythritol Esters Probed by Monte Carlo Simulations

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The next generation of eco-friendly refrigerants requires not only excellent thermal performance, environmental compatibility, and high efficiency, but also good miscibility with lubricant oils. Different chemical families with diverse functional groups and architecture have been proposed as lubticant oils for the refrigeration applications, such as polyalkylene glycol (PAG), alkylbenzene (AB), and polyol ester (POE) oils. Due to limited experimental data in the literature, molecular simulation offers a complementary approach to predict reliable thermophysical properties and to provide molecular-level understanding.

In the present work, isochoric-isothermal (*NVT*) Gibbs ensemble Monte Carlo (GEMC) simulations using the Transferable Potentials for Phase Equilibria–United Atom (TraPPE–UA) force field are performed to predict the vapor–liquid coexistence curves and critical properties of pentaerythritol esters (PEC), that act as the main precursors in POE lubricants. The simulation data indicate that the TraPPE–UA force field yields very good agreement with available experimental data. In addition, the phase behavior and the solvation structure for CO_2 in PECs are probed by isobaric-isothermal (*NpT*) GEMC simulations. The effect of PEC alkyl tail length on the solubility of CO_2 is also analyzed. The predicted critical properties will also be useful as input parameters for the equation of state modeling and provide certain guidance for developing refrigerant-lubricant systems.