

High Pressure Compressed Liquid Densities of Heptane: Comparison between Experiments, Molecular Simulation and Equation of State

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For process design it is important to have accurately information about the properties of the different fluids presented in the process. An incorrect description of the properties of the fluid could have an important economic impact into the analysis of a process.

Nowadays, molecular simulation is an important tool to obtain fluid properties at different conditions in a predictive way, but it has not been widely used. On the other hand, engineers have used equations of state (EoS) as a tool to predict the properties of a fluid for years. However experimental data is always important because in this way the properties of the fluid are obtained directly and not through a model for the molecule of the fluid. In this work, heptane was selected to compare the volumetric properties obtained by molecular simulation and by equation of state.

Experimental compressed liquid densities of heptane were measured from 313 to 362 K up to 25 MPa by a vibrating tube densitometer, the estimated uncertainty in the experimental determinations was 0.2 kg m^{-3} [1]. At the same conditions, molecular simulations for this fluid have been carried out to compare the accuracy of the values obtained by this method. Two equations of state has been selected represent the volumetric properties of heptane the PC-SAFT EoS [2] and a new proposed EoS based on the Lennard-Jones potential. Results obtained by the three different methods are discussed.

[1] A. Zuñiga-Moreno, and L.A. Galicia-Luna, J. Chem. Eng. Data **50**, 1224 (2005).

[2] J. Gross, and G. Sadowski, Ind. Eng. Chem. Res. **40**, 1244 (2001).