Experimental Measurements and Molecular Simulations of Density, Derivative Properties, and Viscosity of n-Hexane + n-Dodecane and n-Hexane + Diphenylmethane Binary Mixtures

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Asymmetric mixtures of hydrocarbons are widely present in many oil and gas processes. Consequently, the thermophysical characterization of those asymmetric mixtures is of primary importance in order to optimize oil production and processing. Thus, we designed a set of experimental measurements and molecular simulations of thermophysical properties such as the density, the isothermal compressibility, the thermal expansivity, the heat capacity, the sound speed, and the viscosity on model asymmetric mixtures to test existing and new models on well controlled systems. In a first step, we have investigated two binary mixtures: n-hexane + n-dodecane and n-hexane + diphenylmethane. Density measurements were carried out using an Anton-Paar oscillating U-tube density meter. The sound speed measurements were performed using a pulse transmission-reflection apparatus. The viscosity was measured with an Ubbelohde viscosimeter at atmospheric pressure and with a falling body viscosimeter for higher pressures. Measurements were performed on six sample mixtures ranging from 0 to 100 % of n-hexane, at temperatures from 293.15 to 333.15 K and pressure up to 100 MPa. For molecular simulations, we computed the aforementioned thermophysical properties using classical Molecular Dynamics and Monte Carlo techniques. Two different force fields were evaluated. An in-house coarse grained model based on the Mie chain fluid and a usual fine grained model, the Transferable Potential for Phase Equilibria (TraPPE) united atom force field.