Densities and phase equilibria of supercritical hydrogen, propane and vegetable oil mixtures. Experimental data and thermodynamic modeling

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Heterogeneous catalytic gas-liquid reactions are intensified when carried out in the homogenous fluid phase by means of a supercritical co-solvent. For instance, supercritical propane is used to enhance yield in the hydrogenation of vegetable oils. Besides phase equilibrium knowledge, volumetric information is also needed to elucidate kinetic mechanisms and design continuous supercritical reactors. In this work, we report new experimental *PvT* data of the reactive mixture H_2+sunflower oil + propane. In addition, the phase equilibria and *PvT* data are modeled with the GCA and RK-PR equations of state, respectively. The isochoric method not only provides *PvT* information under the reaction conditions, but also the reactive system compressibility. The *PvT* data of binary and ternary mixtures involving H_2, propane and sunflower oil using the isochoric method cover the (294.8 to 432.5) K temperature range and (2.7 to 24.6) MPa pressure range. In addition, we compare the data with phase envelopes predicted with GCA. Finally, we modeled the new *PvT* data using RK-PR, which is a three-parameter cubic equation of state. Based on correlations of pure component *PvT* behavior, RK-PR predicts accurately the density of binary and ternary mixtures, in spite of the data sensitivity to the mixture composition and global density.. This results can be applied to other similar supercritical hydrogenation systems. The isochoric method not only provides *PvT* information under the reaction conditions, but also the reactive system compressibility, key variable to attain enhanced transport properties.