

An Association Model to Correlate the Experimentally Determined Mixture Solubilities of Methyl 10-Undecenoate with Methyl Ricinoleate in Supercritical Carbon Dioxide

Authors : V. Mani Rathnam, Giridhar Madras

Abstract : Fossil fuels are depleting rapidly as the demand for energy, and its allied chemicals are continuously increasing in the modern world. Therefore, sustainable renewable energy sources based on non-edible oils are being explored as a viable option as they do not compete with the food commodities. Oils such as castor oil are rich in fatty acids and thus can be used for the synthesis of biodiesel, bio-lubricants, and many other fine industrial chemicals. There are several processes available for the synthesis of different chemicals obtained from the castor oil. One such process is the transesterification of castor oil, which results in a mixture of fatty acid methyl esters. The main products in the above reaction are methyl ricinoleate and methyl 10-undecenoate. To separate these compounds, supercritical carbon dioxide (SCCO₂) was used as a green solvent. SCCO₂ was chosen as a solvent due to its easy availability, non-toxic, non-flammable, and low cost. In order to design any separation process, the preliminary requirement is the solubility or phase equilibrium data. Therefore, the solubility of a mixture of methyl ricinoleate with methyl 10-undecenoate in SCCO₂ was determined in the present study. The temperature and pressure range selected for the investigation were T = 313 K to 333 K and P = 10 MPa to 18 MPa. It was observed that the solubility (mol·mol⁻¹) of methyl 10-undecenoate varied from 2.44 x 10⁻³ to 8.42 x 10⁻³ whereas it varied from 0.203 x 10⁻³ to 6.28 x 10⁻³ for methyl ricinoleate within the chosen operating conditions. These solubilities followed a retrograde behavior (characterized by the decrease in the solubility values with the increase in temperature) throughout the range of investigated operating conditions. An association theory model, coupled with regular solution theory for activity coefficients, was developed in the present study. The deviation from the experimental data using this model can be quantified using the average absolute relative deviation (AARD). The AARD% for the present compounds is 4.69 and 8.08 for methyl 10-undecenoate and methyl ricinoleate, respectively in a mixture of methyl ricinoleate and methyl 10-undecenoate. The maximum solubility enhancement of 32% was observed for the methyl ricinoleate in a mixture of methyl ricinoleate and methyl 10-undecenoate. The highest selectivity of SCCO₂ was observed to be 12 for methyl 10-undecenoate in a mixture of methyl ricinoleate and methyl 10-undecenoate.

Keywords : association theory, liquid mixtures, solubilities, supercritical carbon dioxide

Conference Title : ICSF 2019 : International Conference on Supercritical Fluids

Conference Location : Tokyo, Japan

Conference Dates : September 09-10, 2019