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Molecular Representation and Modeling of Renewable Diesel Processing with Canola Oil

ABSTRACT

Process simulation of renewable diesel production processes is required to design and analyze key process units, such as Feed Treatment, HDO and the Hydro-Dewaxing processes. A simulation model was built to correlate the thermodynamic and transport properties of a particular process using canola oil as the feedstock. The model uses commonly identified triacylglycerols (TAGs) to represent the molecular composition of the canola oil. Correlations have been developed with available data to predict the properties for each pure compound, and thereafter the properties of mixture.

Canola oil is typically characterized by analyzing the fatty acids either as free fatty acids (FFA) or as fatty acid methyl esters (FAME) using Gas Chromatography (GC). The slates of canola oil are highly populated with 5 - 8 TAGs with C_{16} - C_{18} long chains, which constitute more than 80% of the total composition. Therefore, the canola oil can be readily represented by a limited number of compounds. In this application, 36 commonly identified TAGs are used in this study to represent the molecular composition of canola oil. The model was developed using Aspen Plus with compositions tuned to match the reported FAME analysis. To estimate the properties of canola oil, the properties of each pure component need to be estimated. Correlations have been developed to estimate the thermal-physical and transport properties of those TAG whose data are not available. The model parameters are based on reported data of several TAGs available in DIPPR database. Model predictions have been validated with reported thermal-physical and transport properties of canola oil. The proposed molecular representation successfully predicted the thermal-physical properties (density and heat capacity), and the transport properties such as thermal conductivity, viscosity, and surface tension of canola oil.

The molecular representation is further applied in the hydro-deoxygenation and hydro-dewax process to produce the renewable diesel from canola oil. The process model is calibrated and validated with available engineering data. The model can be used in similar renewable diesel projects to provide reliable design basis for engineering and operations.