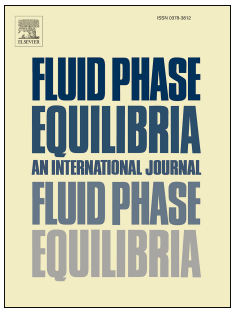
Accepted Manuscript



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PII: S0378-3812(18)30209-7

DOI: 10.1016/j.fluid.2018.05.017

Reference: FLUID 11839

To appear in: *Fluid Phase Equilibria*

Received Date: 26 February 2018

Revised Date: 16 April 2018

Accepted Date: 16 May 2018

Please cite this article as: T.T.X. Nguyen, D. NguyenHuynh, Predicting the phase equilibria of esters/ alcohols mixtures and biodiesel density from its fatty acid composition using the modified group-contribution PC-SAFT, *Fluid Phase Equilibria* (2018), doi: 10.1016/j.fluid.2018.05.017.

Predicting the phase equilibria of esters/ alcohols mixtures and biodiesel density from its fatty acid composition using the modified Group-Contribution PC-SAFT

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ABSTRACT

An empirical approach proposed recently (Fluid Phase Equilibria, 434 (2017) 176-192) to distinguish different isomer molecules is extended in this paper aiming to apply for alkyl-esters. The vapor pressure, saturated liquid density of heavy unsaturated and branched alkyl-ester are predicted using the transferred parameters of groups from n-alkanes, branched alkane, cis-alkenes and alkyl-ester. For pressures up to 2100 bar, density data for esters, ranging from C8:0 to C18:0, with up to two unsaturated bonds, are predicted with deviations inferior to 3%.

Different binary ester + ester systems were investigated. Furthermore, the VLE of methanol/ ethanol + ester mixtures are predicted using a transferable cross-association parameters approach. The general agreement between mg-SAFT and experimental data is very good (within 2-3% deviation on pressure).

Finally, in order to validate the predictive ability of the model to be applied in the biodiesel groundwork, the mg-SAFT was then applied to predict the liquid density of 74 biodiesel mixtures based on its fatty acid ester composition. Overall average prediction errors at atmospheric pressure data were 0.71% for 64 multi-component mixtures, and that of 1.36% compared to experimental data for 10 biodiesel systems at high pressure up to 1300 bar.

Keywords

mg-SAFT, LLE, VLE, biodiesel, prediction, high pressure, cross-association

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