



Experimental measurement and prediction of (liquid + liquid + liquid) equilibrium for the system (*n*-hexadecane + water + triacetin)



Emmanuel D. Revellame^{a,1}, William E. Holmes^{a,1}, Rafael Hernandez^{a,*,1}, W. Todd French^a, Allison Forks^a, Taylor Ashe^a, L. Antonio Estévez^{b,*}

^a Dave C. Swalm School of Chemical Engineering, Mississippi State University, MS 39762, United States

^b Department of Chemical Engineering, University of Puerto Rico, Mayagüez, PR 00681, United States

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ABSTRACT

The phase diagram for the ternary system containing (*n*-hexadecane + water + triacetin) was obtained experimentally at $T = 296.15$ K and ambient pressure. Results show that this system is of Type 3 according to the Treybal classification of ternary system. NRTL and UNIQUAC interaction parameters were calculated from binary phase equilibrium values and were used to predict the (liquid + liquid + liquid) equilibrium (LLLE) region. Results indicated that both NRTL and UNIQUAC could predict the LLLE region of the system with similar precision as indicated by the comparable standard deviations. This indicates that the enthalpic contribution to the activity coefficient is predominant and entropic contributions can be neglected.

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1. Introduction

The successful utilization of microbial lipids for various applications, including bioenergy and sustainable chemical platform, is hampered by huge amount of water in which these microbes are cultivated. The water is commonly removed by a combination of centrifugation and evaporation, which has proven not to be an economical option [1].

In a previous study, Revellame *et al.* [2] established a ternary phase diagram for (*n*-decane + water + triacetin) for designing more economical lipid extraction options in the presence of water using fuel-compatible solvent. They modeled the system using NRTL (Non Random, Two-Liquid) equation and concluded that the ternary behavior of the system can be satisfactorily predicted from binary phase equilibrium data alone. This is a good indication that more tedious phase equilibrium studies of systems containing (alkane + water + lipid) can be avoided. If proven true, it would be beneficial for researchers in the field as they go deeper in the

search for the right solvent that could extract specific lipid or class of lipids from microbial sources.

This study was conducted to establish another phase diagram in a continuous effort to find a cost-effective route to lipid extraction from aqueous media. Triacetin was used as the model lipid compound and a fuel-compatible solvent (hexadecane) in the higher diesel fuel range (C_9 – C_{20}) [3] was chosen. Binary phase equilibrium data were used to predict ternary behavior using NRTL and UNIQUAC (universal quasi-chemical) models for activity coefficients. Furthermore, in an effort to compare the NRTL and UNIQUAC models, experimental values for another Type 3 system obtained from literature [4] were also analyzed.

2. Experimental

2.1. Materials

Table 1 shows sources, basic specifications, and some properties of the materials used in this study. All chemicals were used as received from suppliers.

2.2. Mixture preparation

Mixtures (about 5 g) of triacetin, water, and hexadecane covering the entire mass composition space were prepared. The

* Corresponding authors. Tel.: +1 337 482 6062; fax: +1 337 482 1220 (R. Hernandez). Tel.: +1 787 832 4040; fax: +1 787 265 3818 (L.A. Estévez).

E-mail addresses: rah7653@louisiana.edu (R. Hernandez), antonio.estevez@upr.edu (L.A. Estévez).

¹ Present address: Department of Chemical Engineering, University of Louisiana at Lafayette, LA 70504, United States.

TABLE 1
Materials used in this study.

Chemical name	IUPAC name	CAS No.	Source	Supplier code	Mass fraction ^a	Specific gravity ^a
<i>n</i> -Hexadecane	Hexadecane	544-76-3	Sigma–Aldrich	296317	≥ 0.99	0.773
Water	Oxidane, water	7732-18-5	Fisher Scientific	W6	>0.99	1.0
Triacetin	1,3-Diacetyloxypropan-2-yl acetate	102-76-1	Sigma–Aldrich	525073	0.99	1.16 (25 °C)

^a Supplier provided properties.

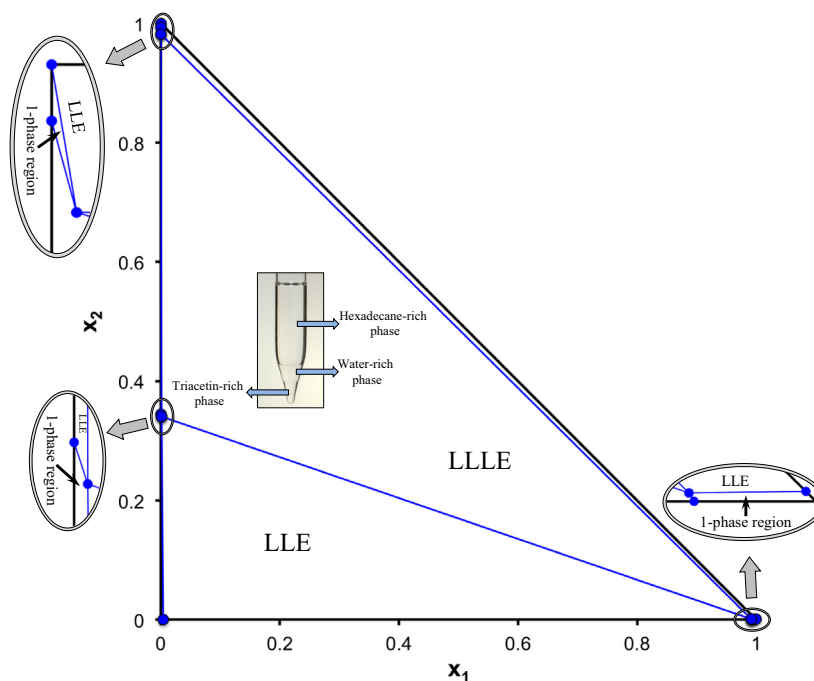


FIGURE 1. Experimental phase diagram for the system {*n*-hexadecane (1) + water (2) + triacetin (3)} at $T = 296.15$ K and atmospheric pressure ($P = 0.1$ MPa).

mixtures were homogenized by vortex-mixing (pulse-mode) at 3000 rpm for 15 min. After centrifugation at 3000 rpm for 15 min, the mixtures were equilibrated at $T = 296.15$ K in a Model 304 Isotemp[®] incubator (Fisher Scientific, Pittsburgh, PA, USA). After at least 1-week equilibration, phases were separated using 2-mL syringes (equipped with 16 g × 5 in needles) and analyzed for triacetin, water, and hexadecane, as described below.

2.3. Sample analyses

Analyses of mixture composition were conducted following the procedure presented by Revellame and co-workers [2]. Triacetin and hexadecane were analyzed using a Varian CP-3800 Gas Chromatograph (GC) (Varian Inc., Palo Alto, CA, USA) equipped with a 15 m (+5 m Guardian) ZB-5HT Inferno column [0.32 mm I.D., 0.10 μm film thickness] (Phenomenex, Torrance, CA, USA). The injector, which was running at 30:1 split ratio, was set at 400 °C while the flame ionization detector was set at 300 °C for the duration of the analysis. The GC oven was set at an initial temperature of 50 °C for 1 min, and then ramped to 180 °C at 18 °C per minute and was set at 180 °C for 1.78 min. Analysis of water was done using a 756 KF coulometer with generator electrode (without diaphragm) equipped with 703 Ti stand (Metrohm, Houston, TX, USA).

2.4. Phase equilibrium values

Experimental binary and ternary phase equilibrium values included at least 8 results for each binary sub system and 7 ternary

LLLE systems. Based on the Treybal classification, the system (*n*-hexadecane + water + triacetin) belongs to the Type 3 ternary system [5] as seen in figure 1 with values given in table 2. The general features of this system are similar to those of the (*n*-decane + water + triacetin) system [2].

3. Data correlation

3.1. NRTL and UNIQUAC

Although a previous study showed that NRTL can satisfactorily predict the ternary phase behavior of the (*n*-decane + water + triacetin) system using only binary sub-system data [2], UNIQUAC was also considered in this study for two reasons: (1) it uses surface fraction instead of mole fraction as primary concentration variable, and (2) NRTL is just an enthalpic model, while UNIQUAC includes both enthalpic contributions (associated with the residual terms to account for interaction energy) and entropic contributions (associated with the combinatorial terms to account for molecular size and shape) [7,8]. These indicate that UNIQUAC could be the more suitable model for mixtures containing small or large molecules as for the case of the system considered in this study (water + lipid mixture).

In 1978, Anderson and Prausnitz modified the UNIQUAC model by empirically adjusting the surface area parameter of the model. The modification showed better correlation for systems containing water and lower alcohols suggesting a significant role of hydrogen

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