

# Liquid–liquid and liquid–liquid equilibrium for ternary system water–acetonitrile–cyclohexene at 298.15 K



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## ARTICLE INFO

### Article history:

Received 18 February 2015

Received in revised form

16 June 2015

Accepted 25 June 2015

Available online 2 July 2015

### Keywords:

Liquid–liquid equilibrium

Liquid–liquid

equilibrium

Azeotropic systems

## ABSTRACT

Liquid–liquid (LLE) and liquid–liquid equilibrium (LLE) data for the ternary system water–acetonitrile–cyclohexene were obtained at 298.15 K and 99.06 kPa. The results of mathematical modelling of LLE and LLE with the use of the NRTL and UNIFAC models were compared. Both models provide a good description of vapour–liquid equilibrium (VLE). It was determined that the experimental and calculated (NRTL) data are in good agreement, and it was demonstrated that the UNIFAC model could not be used for studying LLE and LLE in the considered system.

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## 1. Introduction

The investigation of phase equilibrium in multicomponent multiphase systems is a complex task. One of the most effective methods of studying these is through mathematical modelling. There are several research studies devoted to development of algorithms for LLE and LLE calculation, correlation and prediction [1–3]. The authors agree on the use of the NRTL model for the description of the phase equilibrium of multiphase systems. The parameters of the NRTL model should give both correct qualitative reproduction of the thermodynamic behaviour of the system and quantitative agreement with experimental data. However, experimental LLE data are scarce compared with the VLE and LLE data. An analysis of the literature revealed approximately 60 experimentally-studied ternary systems. Currently, the systems most investigated are those containing water [4–12].

At the same time, the research of splitting systems is highly promising from the point of view of separation processes. Recently, the number of works devoted to development of three-liquid-phase extraction for the separation of complex mixtures has increased [13–19]. The use of the splitting effect is analogous to separation processes based on distillation methods [20,21] because

it is spontaneous and does not require additional energy costs. Thus, the investigation of the liquid–liquid envelope is necessary for the design of separation processes.

In the present study, the water–acetonitrile–cyclohexene system, which is an industrially important system for the synthesis of cyclohexanone [22]), was chosen as the object of a splitting-diagram study. There are number of experimental studies that present VLE and LLE data for the binary constituents of a ternary system. The binary systems water–acetonitrile and water–cyclohexene contain azeotropes with minimum boiling temperatures [23–27]. The water–acetonitrile system is homogeneous, and the other two are heterogeneous [28–29].

An analysis of the published data indicates that there are no experimental data for the liquid–liquid and liquid–liquid equilibrium in the considered ternary system. This work presents the results of our experimental study of LLE and LLE in the water–acetonitrile–cyclohexene system at 298.15 K and 99.06 kPa.

## 2. Experimental

### 2.1. Materials

The purities of the chemicals (see Table 1) were verified chromatographically and in terms of refraction indexes. All physico-chemical constants of the pure substances were determined to be in agreement with the data in the literature [30]. The cyclohexene

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**Table 1**  
The purities of the chemicals.

Substance	Purity, mass fraction	Manufacturer
Water	0.999	–
Acetonitrile	0.999	LAB-SCAN analytical sciences
Cyclohexene	0.990	ACROS ORGANICS

**Table 2**  
Experimental (liquid + liquid + liquid) data for the system water–acetonitrile–cyclohexene for mole fractions ( $x$ ) at temperature  $T = 298.15$  K and pressure  $p = 99.06$  kPa.<sup>a</sup>

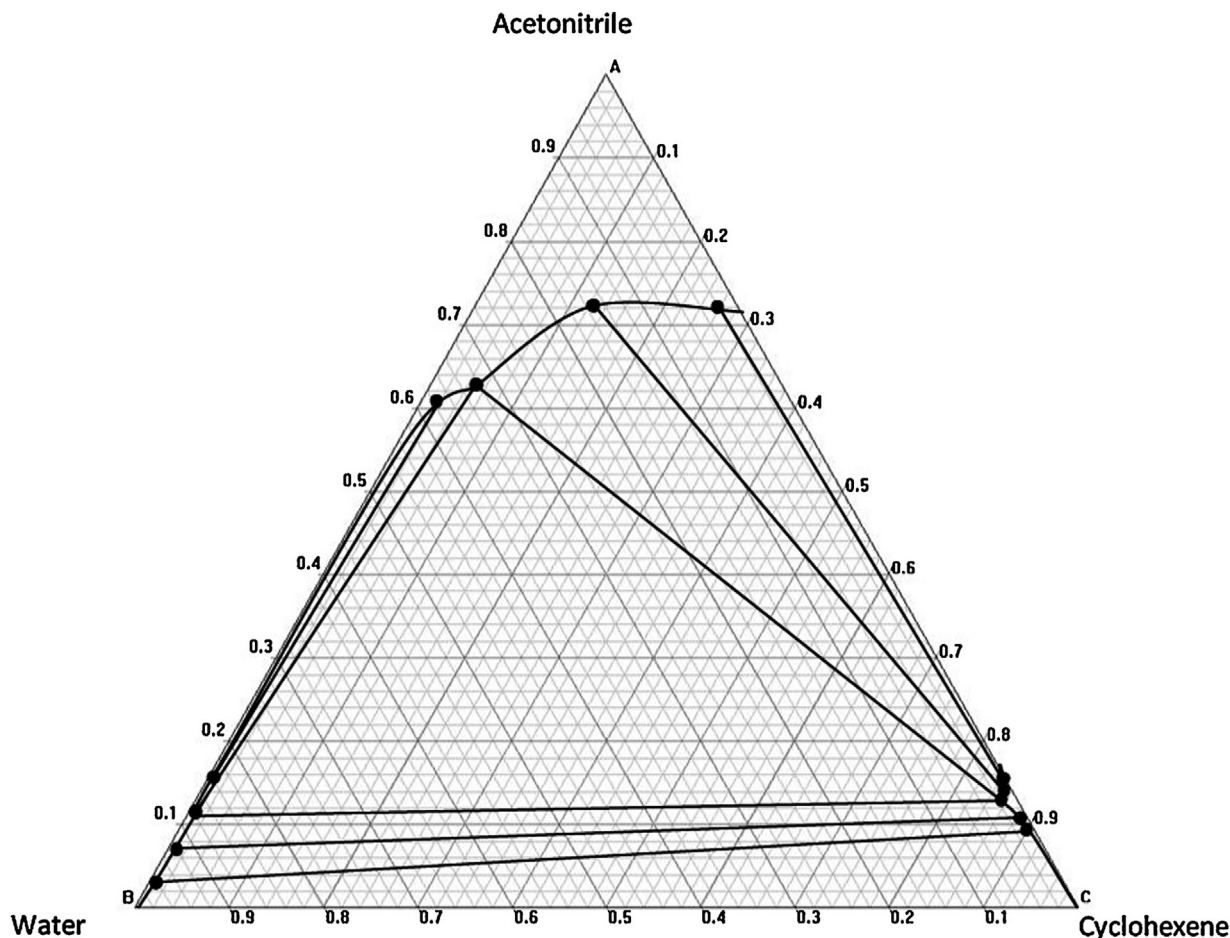
Composition of coexisting phases, mole fraction					
Phase 1		Phase 2		Phase 3	
Water	Acetonitrile	Water	Acetonitrile	Water	Acetonitrile
0.894	0.103	0.321	0.620	0.009	0.116

Standard uncertainties are  $u(T) = \pm 0.3$  K,  $u(x) = \pm 0.0032$ , and  $u(p) = \pm 0.4$  kPa.

**Table 3**  
Experimental (liquid + liquid) data for the system water–acetonitrile–cyclohexene for mole fractions ( $x$ ) at temperature  $T = 298.15$  K and pressure  $p = 99.06$  kPa.<sup>a</sup>

Composition of coexisting phases, mole fraction			
Phase 1		Phase 2	
Water	Acetonitrile	Water	Acetonitrile
0.968	0.031	0.013	0.096
0.931	0.068	0.004	0.099
0.851	0.148	0.338	0.602
0.013	0.135	0.017	0.720
0.017	0.136	0.151	0.728

Standard uncertainties are  $u(T) = \pm 0.3$  K,  $u(x) = \pm 0.0032$ , and  $u(p) = \pm 0.4$  kPa.



**Fig. 1.** Splitting diagram of the water–acetonitrile–cyclohexene ternary system.

was purified by distillation and chromatographic analysis indicated that its purity practically did not change. The water was double-distilled.

## 2.2. Methods

The LLE and LLE were investigated using gas chromatography. Ternary mixtures of known composition within the splitting region were prepared by the gravimetric method using a SciencTech SA210 analytical balance with an accuracy of 0.0001 g. It was considered that the phase equilibrium is reached when there was a full distribution of phases among themselves. After phase equilibrium was reached the phases were separated using a separatory funnel and were analysed by gas chromatography. A LChM-80 chromatograph (Russia) was used with two packed columns, a Porapak Q (3 m) and a Porapak P (1 m), both with a 3 mm i.d. The column and injector temperatures were 453 K, and the detector temperature was 473 K.

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