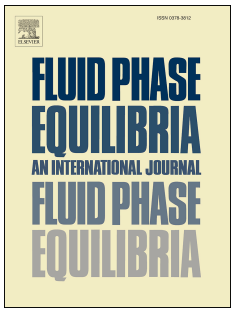

Experimental study of the LL, VL and VLL equilibria of water + 1-butanol + 2-octanol at 101.3 kPa

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Experimental study of the LL, VL and VLL equilibria of water + 1-butanol + 2-Octanol at 101.3 kPa

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ABSTRACT

Equilibrium data for the water + 1-butanol + 2-octanol system is determined in this work. Liquid-liquid equilibrium (LLE) data are obtained at 303.15K and 313.15K, with a view to investigating the influence of temperature.

Vapour-liquid-liquid equilibrium (VLLE) and vapour-liquid equilibrium (VLE) data of the same system are also determined at 101.3 kPa, by means of a modified Fisher Labodest recirculating still that is coupled to an ultrasonic probe. Additionally, the heterogeneous binary azeotrope of the pair water + 2-octanol is determined.

Correlation parameters are obtained from the experimental results for use in the universal quasichemical (UNIQUAC) and non-random two-liquid (NRTL) thermodynamic models in CHEMCAD 7. The UNIQUAC, NRTL and original universal functional group activity coefficient (UNIFAC) models are then, in turn, used to predict the LLE and VLLE data from these correlation parameters.

KEYWORDS

Water, 1-butanol, 2-octanol, liquid-liquid, vapour liquid, vapour-liquid-liquid

1.- INTRODUCTION

Butanol is a fuel of natural origin that is gaining great relevance at the moment due to the advantages it displays with respect to ethanol.

Now that butanol is becoming a substitute for bioethanol, companies are trying to develop other methods of producing it that differ from the traditional ABE (Acetone-Butanol-Ethanol) fermentation. Yet other usual industrial production methods are often the Oxo process and Guerbet reaction [1].

It is for this reason that the Spanish company Abengoa undertook a technological development project in 2013 that converts bioethanol, already produced by the company, into butanol by means of the catalyzed Guerbet reaction [1]. This reaction obtains longer molecular chains from others involving shorter chains, via a catalytic dimerization.

Since this dimerization is not selective, other alcohols (C3-C8) may appear that can adversely affect the subsequent purification processes of butanol, because the existing equilibria between phases can be modified by the various species that are present. Based on this fact, it would be desirable to have access to equilibrium data for butanol in the presence of those long chain alcohols.