Isobaric Vapor Liquid Equilibria of Systems containing N-Alkanes and Alkoxyethanols

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1. Introduction

Surfactants are industrially important materials because of various applications in the cosmetic, pharmaceutical, and food industries. For successful usages of these materials in the process design and operation, it is essential that phase behaviors for mixtures containing nonionic surfactant systems, such as vapor-liquid equilibria and liquid-liquid equilibria are accurately measured. Ethoxylated alcohol {H-(CH2)i-(OCH2CH2)j-OH or CiEj} surfactants are a particularly interesting class of substances because that they have both ether (O) and hydroxyl (OH) groups in the one molecule. There are many phase equilibrium data for Water + surfactant measured at atmospheric pressure, but few data are available for hydrocarbon + surfactant systems.

In this study, we measured (vapor + liquid) equilibrium data for {n-hexane + 2-isopropoxyethanol (i-C3E1) } and {n-heptane + 2-isopropoxyethanol (i-C3E1)} systems at pressures ranging from (60 to 100) kPa. VLE data of binary systems were found to be thermodynamically consistent. In addition, the experimental data were correlated with using the three suffix Margules, Wilson, NRTL, and UNIQUAC equations for the liquid phase activity coefficients.

2. Experimental

2.1. Materials.

n-heptane and *n*-hexane were supplied by Junsei Chemical (Japan) with a minimum purity of 99.5 % (GC) and stored over a molecular sieve. 2-isopropoxyethanol was supplied by Aldrich (U.S.A) with a minimum purity of 99.0 % (analytical grade). We maintained the chemicals at a slightly higher pressure than the vapor pressure of each chemical for the degassing purpose before the experiments.

2.2. Apparatus and Procedures.

Experiments were conducted using the apparatus VLE 602 of the company i-Fischer Engineering GmbH, Waldbuettelbrunn (Germany). This apparatus's equilibrium vessel is an all-glass dynamic-recirculating still. And the Cottrell pump in the still ensures that liquid and vapour phases are sufficiently mixed and two phases' temperatures are measured by temperature sensing element. The accuracy of the temperature measuring system was ± 0.01 K in the range, as specified by the manufacturer. Pressure was measured with a Fischer digital manometer with a precision of ± 0.01kPa.

In each experiment, the desired operating pressure was adjusted at the controller and the heating system was turned on. When the temperature and pressure are remaining constant for a time period of 30min or longer, equilibrium conditions were assumed. Samples were taken with using syringes and analyzed by the gas chromatography (GC). The GC was equipped with a thermal conductivity detector (TCD) and a Porapak Q column (1.83-m long; 3.18-mm diameter; mesh range, 80/100). Helium was used as a carrier gas.

3. Results and Discussion

The isobaric VLE data were measured at 60, 80, and 100kPa. These data for the system n-hexane (1) + 2-isopropoxyethanol (2) and n-heptane (1) + 2-isopropoxyethanol (2) are illustrated in the tables and the figures. The vapor pressures of pure components were obtained by the Antoine equation. The correlation of the equilibrium data was carried out with the several models (the three suffix Margules, Wilson, NRTL, and UNIQUAC) for the activity coefficient and the two-term virial equation for the fugacity coefficient. The pure parameters of n-hexane and n-heptane (area parameter q and volume parameter r) needed for UNIQUAC were taken from

DIPPR Database. For 2-isopropoxyethanol, they were obtained from the method of Abrams and Prausnitz.

The comparison of phase diagrams between the experimental data and the calculated values are shown in the two figures. The calculated results give a good agreement with the experimental data at each pressure. Minimum boiling azeotrope is present in the system n-heptane (1) + 2-isopropoxyethanol (2).

4. Conclusions

The isobaric VLE data for *n*-hexane + 2-isopropoxyethanol and *n*-heptane + 2-isopropoxyethanol systems were obtained at 60kPa, 80kPa, and 100kPa. Four activity coefficient models, namely, three suffix Margules, Wilson, NRTL, and UNIQUAC, were used for correlations. Correlation results are in good agreement with the experimental data. The system n-heptane + 2-isopropoxyethanol shows the azeotropic composition.

FIGURE CAPTIONS

FIGURE **1**. Experimental Data for the system *n*-hexane (1) + 2-isopropoxyethanol (2) at 60, 80, and 100 kPa : ●, 100kPa; △, 80kPa; ◇, 60kPa; solid curves, UNIQUAC model; medium-dashed curves, NRTL model, dashed-dot curves, Wilson model; dotted curves, Margules equation.

FIGURE **2**. Experimental Data for the system *n*-heptane (1) + 2-isopropoxyethanol (2) at 60, 80, and 100 kPa : ●, 100kPa; △, 80kPa; ◇, 60kPa; solid curves, UNIQUAC model; medium-dashed curves, NRTL model, dashed-dot curves, Wilson model; dotted curves, Margules equation.
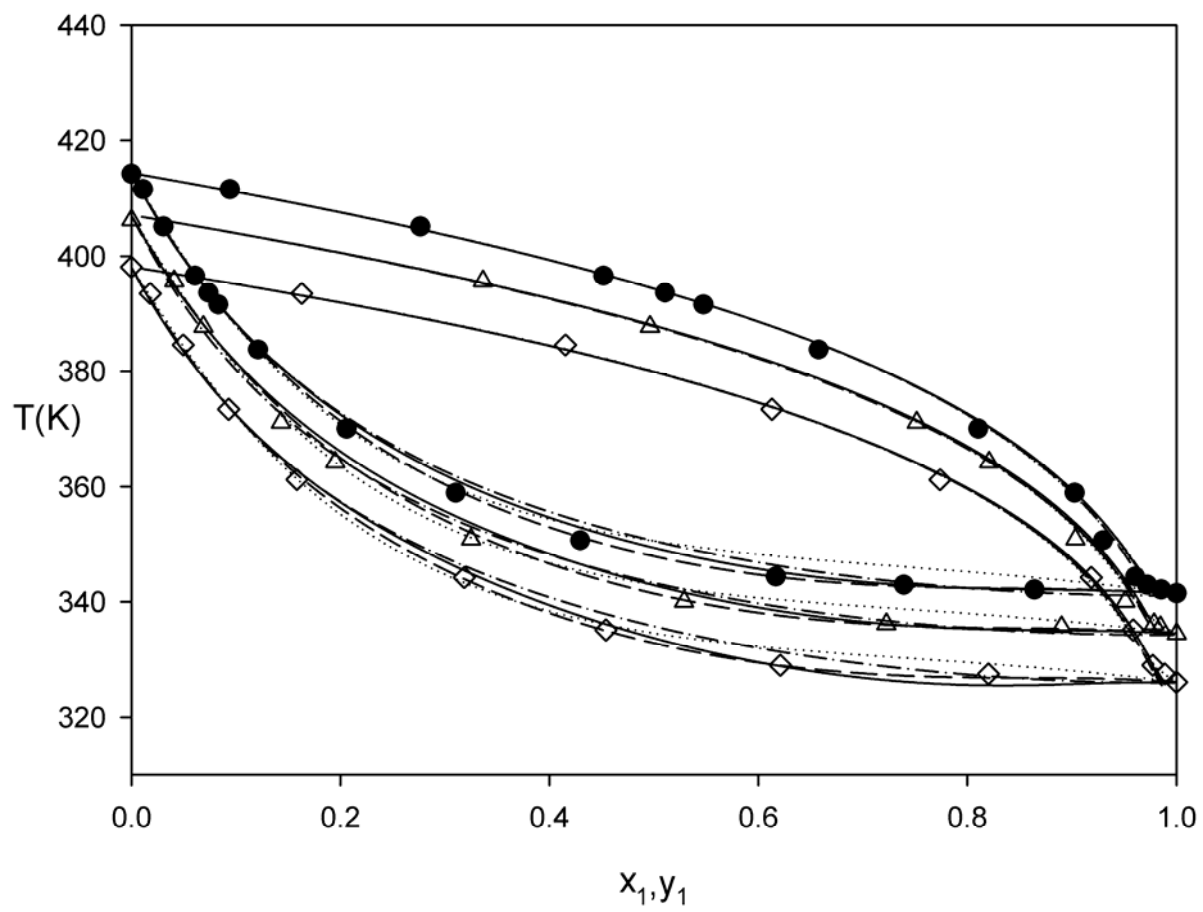
Figure 1.

Figure 2.