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Short communication

Solubility of 1,4-butanedioic acid in aqueous solutions of ethanol or 1-propanol

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ABSTRACT

The solubilities of 1,4-butanedioic acid in some pure solvents and in binary mixtures of water–ethanol and water–1-propanol were determined by the static analytical method at temperatures between 293.2 K and 333.2 K. It was observed that there is a maximum acid solubility in all systems tested. The results obtained for the dicarboxylic acid in pure solvents are in good agreement with the experimental solubility data available and their dependence with the temperature. The experimental data can be well correlated by an empirical equation.

1. Introduction

Carboxylic acids have industrial application directly or indirectly through acid halides, esters, salts, and anhydride forms, polymerization, etc. Dicarboxylic acids can yield two kinds of salts or esters, as they contain two carboxyl groups in one molecule. It is useful in a variety of industrial applications include: plasticizer for polymers, biodegradable solvents and lubricants, engineering plastics, epoxy curing agent, adhesive and powder coating, corrosion inhibitor, perfumery and pharmaceutical and electrolyte.

There is almost infinite number of esters obtained from carboxylic acids. Amongst carboxylic acids available by fermentation, 1,4-butanedioic acid and its derivatives have enormous potential as commodities in the chemical market [1–5]. 1,4-Butanedioic acid (or succinic acid) is a dicarboxylic acid of four carbon atoms. It occurs naturally in plant and animal tissues. It is a white powered crystal produced as an intermediate of the tricarboxylic acid cycle and also as one of the fermentation products of energy metabolism [6,7]. The versatile properties of 1,4-butanedioic acid make it an important ingredient in the manufacture of various specialty and commodity chemicals [8–11]. It is purified by crystallization in the final production step [12].

To select the proper solvent and to design an optimized separation process, it is necessary to know its solubility in different solvents. According to the literature [13–15], few solubilities of 1,4-butanedioic acid in pure solvents and mixtures have been reported [15–17]. In this work, the solubilities of 1,4-butanedioic acid in mixtures of water–ethanol and water–1-propanol were experimentally determined using a gravimetric method. Literature has been suggested, for systems containing acids, two empirical equations to correlate the binary SLE data. Then, the ones were adopted in this study to choose the most suitable to predict the SLE for the systems. These results have shown that for pure solvents it is hardly recommended exponential model. However, polynomial equation is more appropriate for mixtures.

2. Experimental

2.1. Materials

A white crystalline powder of 1,4-butanedioic acid (CAS no. 110-15-6) (Powder X-ray Diffraction of the starting material confirmed that this was the 1,4-butanedioic acid referred to the CCDC reference SUCACBO2) was obtained from VETEC Chemical Reagent Ltda. (Brazil). The mass fraction purity is greater than 0.99. It was used without further purification. The ethanol and 1-propanol used in the experiments were of analytical reagent grade with mass fraction purities greater than 0.99. Deionized and bidistilled water was prepared in our laboratory. Table 1 summarizes the materials information.

2.2. Apparatus and procedures

Solubility was measured by a static method [9–11,16]. The apparatus for the solubility measurement and the procedure are the same as those described in the literature [12]. The solubility apparatus consisted of a volume of a 45 mL jacketed glass vessel maintained at a desired temperature by water circulated from

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Table 1
Sources and mass fraction purity of the materials.

Chemical name	Source	Purification method	Mass fraction purity
1,4-Butanedioic Acid	VETEC Chemical Reagent Ltda.	None	>0.99
Ethanol	ISOFAR	None	>0.99
1-Propanol	ISOFAR	None	>0.99

a water bath with a digital thermoelectric controller (Nova Ética, Brazil). The jacket temperature could be maintained within (0.1 K) of the required temperature. A mercury-in-glass thermometer with an uncertainty of ±0.1 K was inserted into the inner chambers of the vessels for measurement of the solution temperature. Continuous stirring was achieved with a magnetic stirrer. A condenser was connected with the vessels to prevent the solvents from evaporating. Masses of solute and solvent were weighed using an analytical balance (Bioprecisa, Brazil) with an accuracy of ±0.1 mg. First, predetermined known masses of 1,4-butanedioic acid and solvent were transferred in the jacketed vessel. Then the contents of the vessel were stirred until the temperature fluctuation varied by less than 0.1 K, and a suitable dose of solute was added so that it did not exceed the solubility too much. Then the mixture was stirred for 2 h. When the portion of solids has not disappeared, the stirrer was turned off and 4 h of decanting started. Two or three liquid samples (5 mL) were withdrawn and left in the oven until constant weight. The saturated solubility of solute (S) could be obtained with the accuracy of sample composition about of ±0.12 g of acid/100 g of solution.

In tables, x (±0.0001) and S represent mole fraction of alcohol and solubility of the acid (in g of acid/100 g of solution), respectively. All the experiments were repeated three times at each temperature, and estimated absolute deviations (δ) of the experimental values are informed in Tables 2, 4 and 5.

3. Results and discussion

The results of 1,4-butanedioic acid solubility in water in different temperatures determined in this work and by other researchers are listed in Table 2. It can be seen that our data are more consistent with the newest [15] literature data. Table 2 shows that the maximum deviation of the solubilities of 1,4-butanedioic acid in water in this work and in the literature from experimental values is less than 3%.

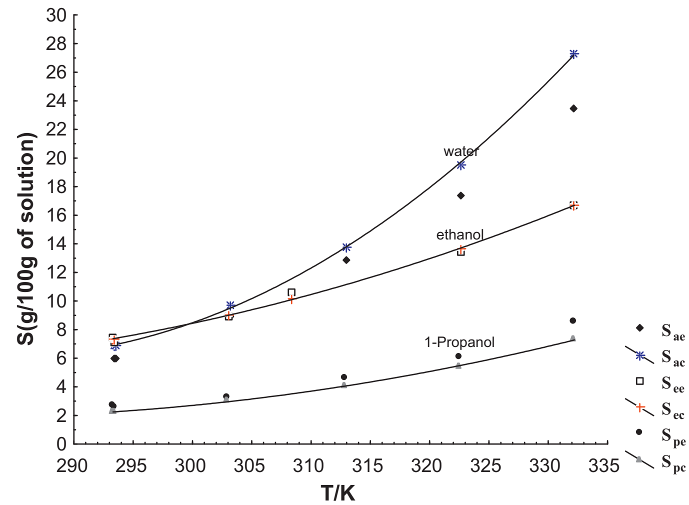

Fig. 1. Solid–liquid phase diagram for the binary systems of 1,4-butanedioic acid + pure solvent (water (⧫); ethanol (□); 1-propanol (●)).

The solubility of 1,4-butanedioic acid (S) in pure solvent as function of temperature (T) can be correlated by the following polynomial (S_P) and exponential (S_E) equations [18,19]

$$S_P = a + bT + cT^2 \quad (1)$$

$$S_E = a' + \exp(b'T) \quad (2)$$

where a, b, c, a' and b' are the fitted parameters.

Then, for pure solvents, Fig. 1 gives the plot of the solubility of 1,4-butanedioic acid in these solvents at a temperature range of about 293.2–333.2 K. Also, in Fig. 1, the solubilities of 1,4-butanedioic acid in water, ethanol and propanol is represented by the best (exponential) correlation tested.

Table 3 lists the correlated results for the binary systems, indicating that based on the calculated average absolute deviations (AAD) of the solubility polynomial equation is not recommended. The calculated results from this model are compared with the experimental values in Fig. 1. Then, as published by Buchowsky et al. [19] exponential model is capable of representing the behavior of the liquid mixtures for all the investigated binary systems.

All experimental data are included in Tables 4 and 5. In these tables, x is the mole fraction of alcohol and δ is the experimental standard deviation among three samples. Analyzing the data for each temperature, it can be noted that all of them have a maximum point between zero and pure alcohol.

Table 2
Comparison the SLE data of 1,4-butanedioic acid in water (p = 92.4 kPa) with literature (S, g of acid/100 g of solution).

This work			Apelblat and Manzurola (1987)		Lin et al. (2007)	
T/K	S	δ	T/K	S	T/K	S
293.2	5.97	0.048	293.2	6.75	296.3	5.56
303.2	8.91	0.036	303.2	9.58	–	–
313.2	12.84	0.082	313.2	13.80	–	–
323.2	17.33	0.017	323.2	19.44	324.1	18.14
333.2	23.51	0.088	333.2	25.09	–	–

Standard uncertainties u are $u(T)$ = 0.1 K and $u(S)$ = 0.12 g/g.

Table 3
Parameters and average absolute standard deviations for polynomial and exponential equations.

System	a	b	c	σ_P	a'	b'	σ_E
1,4-Butanedioic acid + water	417.368	−3.0367	0.0056	2.5009	0.0002	0.0356	0.8799
1,4-Butanedioic acid + ethanol	124.013	−0.9585	0.0019	1.1225	0.0151	0.0211	0.2626
1,4-Butanedioic acid + 1-propanol	238.263	−1.6469	0.0029	2.5009	0.0003	0.0304	0.6889