Densities, Surface Tensions, and Refractive Indices of the Water + 1,3-Propanediol System

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Densities, surface tensions, and refractive indices of the binary water + 1,3-propanediol system were measured at temperatures of 298.15, 303.15, 308.15, 313.15, 318.15, and 323.15 K and at 1,3-propanediol mass fractions of 0.00, 0.10, 0.20, 0.40, 0.60, 0.80, and 1.00, respectively. The measured data were well correlated with the simple polynomial equations. The average absolute deviations were found to be 0.123% for density, 0.77% for surface tension, and 0.045% for refractive index.

Introduction

Various working fluids have been proposed to satisfy specific conditions required for such systems as air-cooled absorption chillers, low-temperature heat-driven heat pumps, and solar-powered absorption chillers. Thermodynamic and transport properties of working fluids need to be closely examined because these properties play a great role in the successful design and operation of air-cooled absorption chillers. Among many properties, the density and surface tension are basic properties of importance in analyzing heat and mass transfer of working fluids. At a vapor−liquid interface, surface tension, which cannot be calculated from an equation of state, affects the transfer rates of vapor absorption. An experimental refractive index graph can be used as a calibration curve for determining the concentration of an unknown system. This simple method can determine the concentration of a solution exactly with the aid of a precise refractometer.

In a previous paper (Park et al., 1997), we proposed a new working fluid containing 1,3-propanediol in order to overcome the crystallization problem appearing in an air-cooled absorption machine based on pure lithium bromide. Although it is important to investigate elementary mixtures to analyze the effect of each component, no experimental work for the water + 1,3-propanediol system has been reported yet. As a part of our continuing research and to study the interaction among the components of working fluids, densities, surface tensions, and refractive indices of the binary water + 1,3-propanediol system were measured in this work using a pycnometer, the capillary rise method, and an Abbe refractometer, respectively.

Experimental Section

Materials. 1,3-Propanediol, lithium chloride, and lithium bromide (>99.0% purity), all manufactured by Sigma-Aldrich chemical company, were used in this work without further purification. The water used in making all solutions was triple-distilled. Benzene (Junsei Chemical Co. Ltd., >99.5% purity) and methanol (Merck, >99.8% purity) were also used for calibration experiments.

Apparatus and Procedure. A pycnometer was used to measure the densities of binary solution mixtures. The experimental apparatus consisted of a pycnometer, a thermometer (mercury-filled glass thermometer) to measure the temperatures of the solutions, and a water bath to control the temperatures of the solutions.

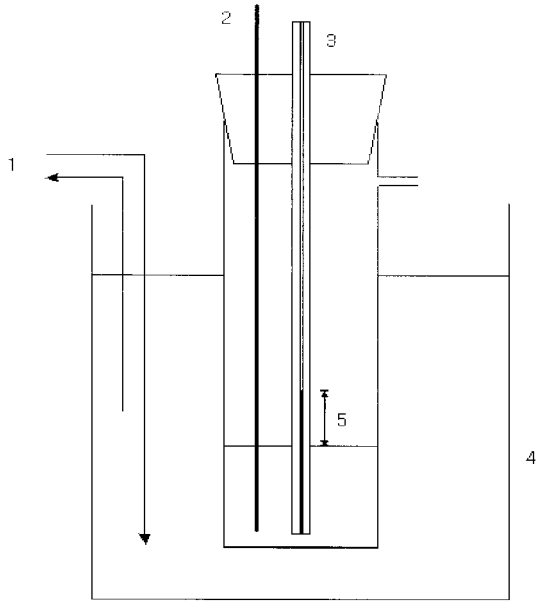

Figure 1. Schematic diagram of experimental apparatus for measuring surface tension: 1, external bath circulator; 2, thermometer; 3, capillary; 4, water bath; 5, capillary rise.

Figure 1 shows the experimental apparatus used for the measurement of surface tension. The whole apparatus consists of a water bath, a bath circulator, a capillary tube, a thermometer (mercury-filled glass thermometer), and a cathetometer. The temperature of a capillary tube was controlled by the bath circulator (JEIO tech. RBC-20) within ±0.1 K. The solution temperature in the capillary tube was measured with the thermometer with an accuracy of ±0.1 K. The height of the liquid rise in the capillary tube was determined with the cathetometer (N.O.W. NCM 30) with an accuracy of 10^{-5} m. The capillary was calibrated with benzene, and a cathetometer was used to measure the capillary rise. In measuring the refractive indices, a precision Abbe refractometer 3T (Atago Co.) was used. An

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Table 1. Densities (ρ) for (1 − *x*)Water + *x*1,3-Propanediol

	ρ/kg·m^{-3}					
x	298.15 K	303.15 K	308.15 K	313.15 K	318.15 K	323.15 K
0.00	997.048	995.651	994.036	992.220	990.130	988.030
0.10	1003.517	1001.926	1000.228	998.159	996.067	993.932
0.20	1010.822	1008.976	1007.112	1004.901	1002.718	1000.537
0.40	1026.260	1023.815	1021.306	1018.597	1015.897	1013.433
0.60	1039.727	1036.927	1033.858	1030.748	1027.769	1024.729
0.80	1048.478	1045.557	1042.548	1039.221	1036.081	1032.808
0.90	1050.341	1047.190	1044.056	1040.754	1037.615	1034.376
1.00	1049.717	1046.718	1043.558	1040.277	1037.517	1034.151

Table 2. Surface Tensions (σ) for (1 − *x*)Water + *x*1,3-Propanediol

	σ/mN·m^{-1}					
x	298.15 K	303.15 K	308.15 K	313.15 K	318.15 K	323.15 K
0.00	71.975	71.200	70.400	69.600	68.770	67.940
0.10	67.137	66.882	66.710	66.409	66.093	65.393
0.20	65.277	65.083	64.591	64.047	63.686	63.473
0.40	62.387	62.102	61.828	61.318	60.930	59.942
0.60	59.328	58.969	58.748	58.190	57.703	57.244
0.80	56.476	56.040	55.771	55.255	54.766	54.287
1.00	53.125	52.679	52.489	52.001	51.556	51.144

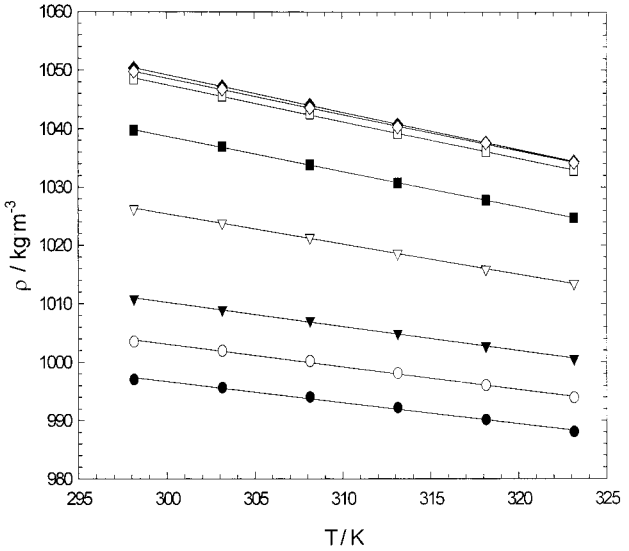

Figure 2. Densities of the water + 1,3-propanediol system at various 1,3-propanediol mass fractions: (●) 0.00; (○) 0.10; (▼) 0.20; (▽) 0.40; (■) 0.60; (□) 0.80; (◆) 0.90; (◇) 1.00; (—) calculated.

external bath circulator was used to control the experimental temperature within ±0.1 K.

Results and Discussion

Density. The measured density data of the binary system were presented in Table 1 and Figure 2. While the mixture density increases with the mass fraction of 1,3-propanediol almost up to 0.8, it changes just a little over 0.8, so the lines are almost overlapped. The density of the solution is linearly decreasing as temperature increases.

Surface Tension. The surface tensions of the water + 1,3-propanediol system were measured in the temperature range from 298.15 K to 323.15 K and the 1,3-propanediol mass fraction range from 0.00 to 1.00, respectively. The surface tension was directly calculated from the following simple equation:

$$\sigma = \frac{1}{2} \cdot h \cdot r \cdot \rho \cdot g \qquad (1)$$

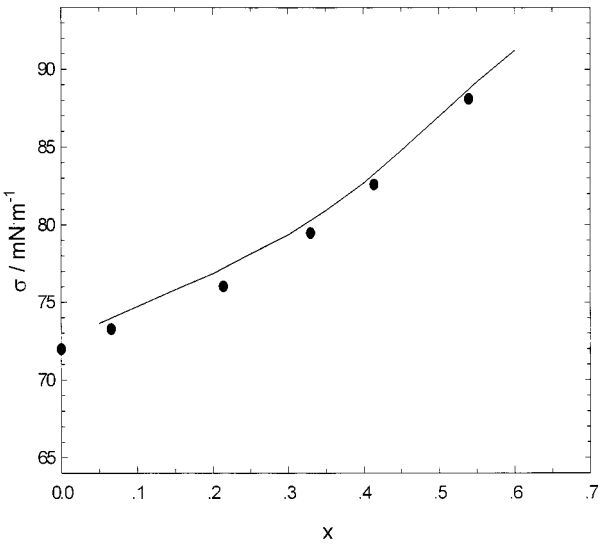

Figure 3. Surface tensions of the lithium bromide + water solution at 298.15 K: (●) this work; (—) Uemura et al.

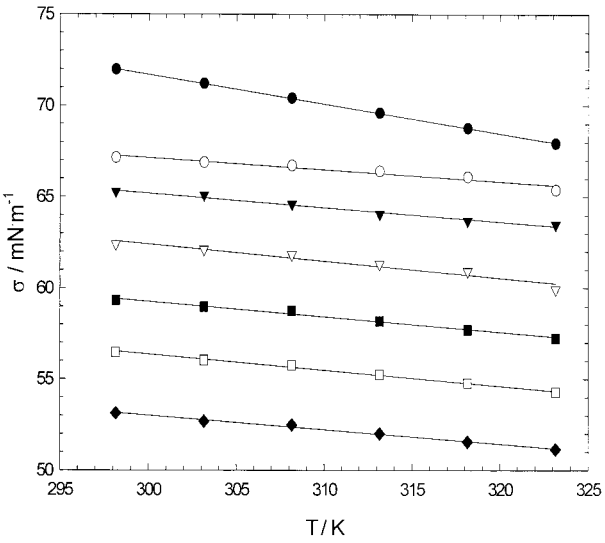

Figure 4. Surface tensions of the water + 1,3-propanediol system at various 1,3-propanediol mass fractions: (●) 0.00; (○) 0.10; (▼) 0.20; (▽) 0.40; (■) 0.60; (□) 0.80; (◆) 0.90; (◇) 1.00; (—) calculated.

Table 3. Refractive Indices (n_D) for (1 − *x*)Water + *x*1,3-Propanediol

	n_D					
x	298.15 K	303.15 K	308.15 K	313.15 K	318.15 K	323.15 K
0.00	1.3325	1.3319	1.3313	1.3306	1.3298	1.3292
0.10	1.3428	1.3422	1.3416	1.3407	1.3401	1.3393
0.20	1.3537	1.3529	1.3522	1.3513	1.3503	1.3494
0.40	1.3760	1.3748	1.3739	1.3730	1.3718	1.3708
0.60	1.3983	1.3972	1.3963	1.3948	1.3939	1.3924
0.80	1.4196	1.4184	1.4172	1.4160	1.4142	1.4132
1.00	1.4382	1.4368	1.4354	1.4340	1.4327	1.4312

where σ is the surface tension, h is the height difference between the capillary and the outer tube meniscus, r is the capillary radius, ρ is the density of the sample, and g is gravitational acceleration. To determine the radius of the capillary tube, the calibration experiment was done using the known surface tension and density of benzene. The radius of the capillary tube was found to be 2.71×10^{-4} m. To check the reliability of the experimental apparatus and procedures used in this study, several test experiments were carried out for water, methanol, a lithium chloride + water solution, and a lithium bromide + water solution at

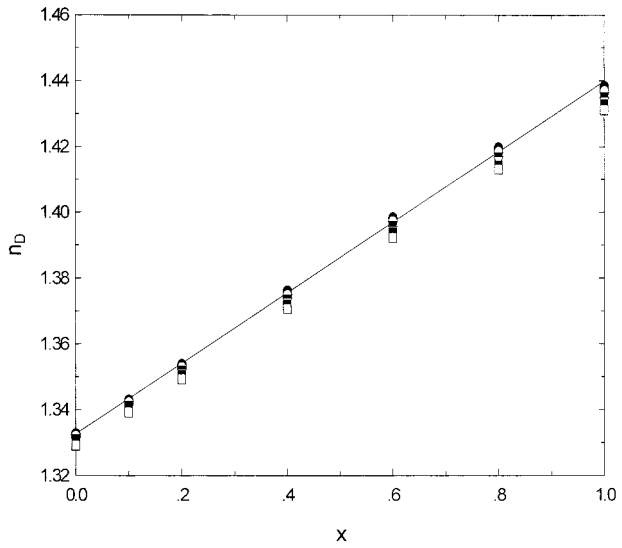

Figure 5. Refractive indices of the water + 1,3-propanediol system at various temperatures: (●) $T = 298.15$ K; (○) $T = 303.15$ K; (▼) $T = 308.15$ K; (▽) $T = 313.15$ K; (■) $T = 318.15$ K; (□) $T = 323.15$ K; (—) calculated at $T = 298.15$ K.

Table 4. Regressed Coefficients Determined from Eq 2

	density		
	A_i	B_i	C_i
$i = 0$	7.40×10	1.95	-3.69×10^{-3}
$i = 1$	1.05×10^3	−5.64	8.16×10^{-3}
$i = 2$	-6.15×10^2	3.46	-5.13×10^{-3}
	surface tension		
	A_i	B_i	C_i
$i = 0$	5.46×10	2.15×10^{-1}	-5.42×10^{-4}
$i = 1$	-4.87×10^2	2.85	-4.36×10^{-3}
$i = 2$	4.76×10^2	−2.92	4.51×10^{-3}
	refractive index		
	A_i	B_i	C_i
$i = 0$	1.30	3.10×10^{-4}	-7.07×10^{-7}
$i = 1$	-9.84×10^{-2}	1.57×10^{-3}	-2.87×10^{-6}
$i = 2$	3.18×10^{-1}	-2.16×10^{-3}	3.58×10^{-6}

various temperatures. The experimental data were compared with the literature values, for water and methanol with the *CRC Handbook* (1995) and for the lithium chloride + water and lithium bromide + water systems with Uemura et al. (Uemura et al., 1964). The experimental surface tension data of the lithium bromide + water system were plotted in Figure 3 along with the literature data. The surface tension data of the water + 1,3-propanediol system were presented in Table 2 and Figure 4. As can be seen in Figure 4, the surface tension of solutions decreased with increasing concentration of 1,3-propanediol, which naturally resulted from the relatively low surface tension of pure 1,3-propanediol.

Refractive Index. The measured refractive indices of the water + 1,3-propanediol system were presented in Table 3 and Figure 5. The refractive index linearly decreased as the temperature increased and linearly increased as the mass fraction of 1,3-propanediol increased.

Regression. For density, surface tension, and refractive index, the measured data were regressed with the following equation using the least-squares method.

$$\rho/\mathrm{kg\cdot m^{-3}} \text{ or } \sigma/\mathrm{mN\cdot m^{-1}} \text{ or } n_D = \sum_{i=0}^{2}[A_i\cdot(\chi/\text{mass fraction})^i + B_i\cdot(\chi/\text{mass fraction})^i\cdot(T/\mathrm{K}) + C_i\cdot(\chi/\text{mass fraction})^i\cdot(T/\mathrm{K})^2] \quad (2)$$

The regressed coefficients were provided in Table 4. The average absolute deviations were found to be 0.123% for density, 0.77% for surface tension, and 0.045% for refractive index. AAD means average absolute deviation and is calculated from the following equation:

$$\mathrm{AAD} = \frac{\sum_{i=1}^{N}\left|\frac{P_{exp} - P_{cal}}{P_{exp}}\right|}{N} \quad (3)$$

where P_{exp} = experimental values, P_{cal} = calculated values, and N = number of points.

Conclusions

The densities, surface tensions, and refractive indices of the water + 1,3-propanediol system were measured at various 1,3-propanediol concentrations and temperatures. The pycnometer was used to measure the densities of binary solution mixtures. The surface tension of this binary mixture was determined by measuring the height difference of the capillary. Also, the data regression was done with simple polynomial equations for each experimental data set. The average absolute deviations (AADs) were found to be 0.123% for density, 0.77% for surface tension, and 0.045% for refractive index.

Nomenclature

AAD = average absolute deviation
g = gravitational acceleration
h = capillary rise
n_D = refractive index
r = capillary radius
T = temperature
x = mass fraction
ρ = density
σ = surface tension

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