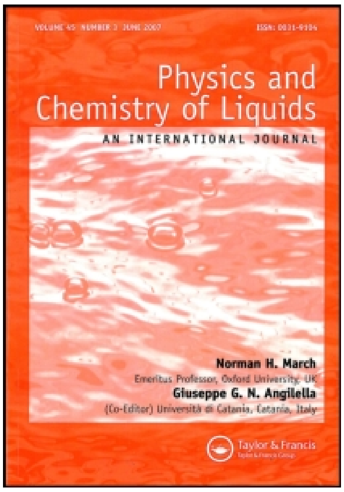

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ISOBARIC VAPOUR–LIQUID EQUILIBRIA IN THE ALLYL ALCOHOL + 1,2-DICHLOROETHANE SYSTEM

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Isobaric VLE are measured at 200, 500 and 705 mm Hg at ten compositions spread evenly, over the entire liquid mole fraction range, emplying a Swietoslawski-type ebulliometer. The *t-x* data collected are found to be well represented by the Wilson model.

KEY WORDS: Vapour-liquid equilibrium, *t-x* relations, boiling point, allyl alcohol, 1,2-dichloroethane.

INTRODUCTION

In continuation of the investigators interest in the phase equilibria of binary mixtures with an alcohol as one component and a chloroethane as the other[1–3], this study on the vapour-liquid equilibria of allyl alcohol + 1,2-dichloroethane mixtures has been taken up. There is no published information on the phase equilibria of this system. The bubble temperature (*t*)-composition (*x*) relations have been measured at 200, 500 and 705 mm Hg, to study the effect of pressure, on the phase equilibrium.

EXPERIMENTAL

A Swietoslawski type ebulliometer, very similar to the one describer by Hala *et al.*[4] is used. Connection of the ebulliometer to a good vacuum system through a mercury manometer, in line facilitated the creation and maintenance of the chosen pressures within ± 1 mm Hg. The equilibrium temperatures are measured to an accuracy of ± 0.1° C, by means of a carefully calibrated mercury-in-glass thermometer. The

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mixtures are prepared gravimetrically and placed in the ebulliometer. The heating rate is adjusted to yield the desired condensate drop-rate of about 30 per minute, as suggested by Hala *et al.*[4] The equilibrium temperature is measured after maintaining the steady drop-rate for sufficient length of time (at least 30 minutes) and the thermometer showed no change in temperature, for at least 15 minutes.

MATERIALS

Allyl alcohol (2-Propen-1-ol) of AR grade procured from SD Fine-Chem. Ltd., Boisar (India), has been distilled twice and the middle fraction of the second distilation is collected for use in the experiments.

1,2-Dichloroethane of AR grade procured from BDH, Bombay (India), is further purified by washing with dilute potasium hydroxide solution and water, dried over phosphorous pentoxide and fractionally distilled twice. The middle fraction of the second distillation is collected for use in the experiments.

A packed column of length equal to 30 theoretical plates is employed for the purification of both substances. Based on the comparison of the physical properties with lilerature[5,6] data, presented in Table 1, the substances are expected to be at least 99.8% pure.

RESULTS AND DISCUSSION

The experimental t-x measurements are correlated using the Wilson equation[7] in the form.

$$\ln \gamma_1 = -\ln[x_1 + \Lambda_{12}x_2] + x_2\left[\frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2} - \frac{\Lambda_{21}}{x_2 + \Lambda_{21}x_1}\right] \tag{1}$$

$$\ln \gamma_2 = -\ln[x_2 + \Lambda_{12}x_1] + x_1\left[\frac{\Lambda_{21}}{x_2 + \Lambda_{21}x_1} - \frac{\Lambda_{12}}{x_1 + \Lambda_{12}x_2}\right] \tag{2}$$

where

$$\Lambda_{12} = \frac{V_2^L}{V_1^L}\exp[-[(\lambda_{12} - \lambda_{11})/RT] \tag{3}$$

Table 1 Physical Properties of Pure Liquids at 293.15 K.

Substance	*Density* $(g{\cdot}ml^{-1})$	*Refractive Index*	*Reference*
Allyl alcohol	0.8523	1.4132	This work
	0.8520	1.4130	5
1,2-Dichloroethane	1.2531	1.4450	This work
	1.2529	1.4451	6

Table 2 Antoine constants of the pure liquids used in this work.

Substance	*A*	*B*	*C*
Allyl alcohol	7.34110	1271.47	188.00
1,2-Dichloroethane	7.15866	1341.37	230.05

and

$$\Lambda_{21} = \frac{V_1^L}{V_2^L} \exp\left[- [(\lambda_{12} - \lambda_{22})/\mathrm{RT}\right] \tag{4}$$

V_1^L and V_2^L are liquid molal volumes and $(\lambda_{12} - \lambda_{11})$ and $(\lambda_{12} - \lambda_{22})$ are the Wilson parameters. λ's are the energies of interaction between the molecules designated by the subscripts. The optimum Wilson parameters $[(\lambda_{12} - \lambda_{11})/\mathrm{R}]$ and $[(\lambda_{12} - \lambda_{22})/\mathrm{R}]$ are obtained by minimizing the objective function ϕ defined as:

$$\phi = \sum [(P_{\mathrm{cal}}/P_{\mathrm{expt}}) - 1]^2 \tag{5}$$

Nelder-Mead optimization technique described in Kuester and Mize[8] is used. Vapour pressures required in the computations are calculated from the Antoine constant given by Dean[9] and reproduced in Table 2 for ready reference. Liquid molal volumes are calculated from Yen and Woods correlation[10]. The values of the optimum Wilson parameters are also noted along with the detailed information on the observed bubble point temperature (t), mole fraction of allyl alcohol in the liquid phase (x_1) and the calculated values of: the mole fraction of allyl alcohol in the vapour phase (y_1), the liquid phase activity coefficients (γ_1 and γ_2), and the excess Gibbs free energy (G^E) in the Table 3. The prospect of formation of azeotropic mixtures at different pressure as shown in Table 4 is predicted based on the model. Experimental investigations confirmed the formation of azeotropes, under the conditions noted in the table. The data and the representation presented in the paper are therefore expected to be reliable within the stated limits of experimental errors.

Table 3 Vapour-Liquid Equilibrium of Allyl alcohol (1) + 1,2-Dichloroethane (2) system. **Wilson Parameters**: $(\lambda_{12} - \lambda_{11})/R = 366.57°\mathrm{K}$; $(\lambda_{12} - \lambda_{22})/R = 132.79°\mathrm{K}$. Standard Deviation in temperature = 0.5°K.

$t\,(°C)$	x_1	y_1	γ_1	γ_2	$G^E\,(J \cdot mol^{-1})$
		Total Pressure: 200 mm Hg			
46.1	0.0000	0.0000	4.1864	1.0000	0
45.1	0.0879	0.1042	3.0499	1.0144	240
44.6	0.1823	0.1649	2.3325	1.0574	528
45.3	0.2599	0.1989	1.9521	1.1119	668
45.6	0.3703	0.2374	1.5933	1.2198	789
46.6	0.4642	0.2681	1.3905	1.3435	827

Table 3 (*Continued*)

$t(^\circ C)$	x_1	y_1	γ_1	γ_2	$G^E (J \cdot mol^{-1})$
		Total Pressure: 200 mm Hg			
46.7	0.5797	0.3109	1.2208	1.5462	795
49.1	0.6840	0.3633	1.1186	1.7922	699
51.3	0.7831	0.4404	1.0542	2.1012	555
56.0	0.8953	0.6071	1.0124	2.5710	301
60.0	0.9574	0.7891	1.0020	2.8987	131
64.3	1.0000	1.0000	1.0000	3.1529	0
		Total Pressure: 500 mm Hg			
70.7	0.0000	0.0000	3.7944	1.0000	0
68.8	0.0879	0.1249	2.8565	1.0131	296
67.9	0.1823	0.1983	2.2314	1.0528	535
69.4	0.2599	0.2395	1.8892	1.1036	679
69.3	0.3703	0.2859	1.5593	1.2048	802
70.3	0.4642	0.3221	1.3698	1.3211	843
70.3	0.5797	0.3711	1.2096	1.5113	811
71.3	0.6840	0.4287	1.1126	1.7411	711
74.4	0.7831	0.5092	1.0514	2.0278	556
78.9	0.8953	0.6700	1.0117	2.4604	305
82.5	0.9574	0.8299	1.0019	2.7607	133
85.9	1.0000	1.0000	1.0000	2.9939	0
		Total Pressure: 705 mm Hg			
81.2	0.0000	0.0000	3.6548	1.0000	0
79.1	0.0879	0.1324	2.7550	1.0126	294
78.6	0.1823	0.2105	2.1932	1.0510	538
78.7	0.2599	0.2544	1.8650	1.1004	681
79.6	0.3703	0.3037	1.5460	1.1991	808
79.2	0.4642	0.3420	1.3617	1.3125	846
80.4	0.5797	0.3931	1.2052	1.4979	817
81.8	0.6840	0.4522	1.1103	2.0000	564
86.5	0.8953	0.6911	1.0115	2.4184	311
91.7	0.9573	0.8429	1.0019	2.7082	146
95.1	1.0000	1.0000	1.0000	2.9332	0

Table 4 Azeotropic conditions.

Pressure (mm Hg)	*Temperature (°C)*	*Mole fraction of Allyl alcohol*
200	45.5	0.1350
500	67.8	0.2050
705	78.6	0.2450

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