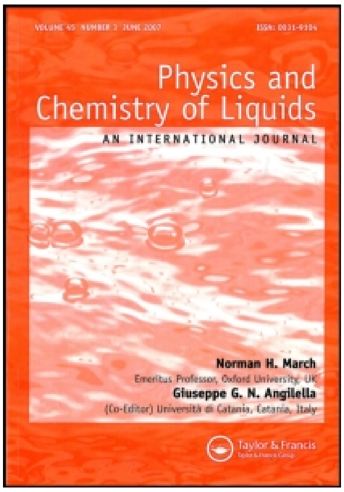

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BUBBLE TEMPERATURE DATA FOR PHENOL-*n*-PROPANOL SYSTEM

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In order to supplement the literature data on VLE, isobaric bubble temperature data were collected for the system phenol-*n*-propanol over the entire composition range by indirect method using a standard Swietoslawski type ebulliometer. The measurements were made at 200, 400 and 710 mm Hg. The experimental $t - x$ data were correlated with both equation of state method and gamma-phi methods. In the former approach the Soave equation of state is used wherfeas in the latter one Wilson, NRTL and UNIQUAC models are used.

KEY WORDS: Equation of state, Soave equation.

INTRODUCTION

Separation of mixtures into useful components or fractions forms one of the most important activities of any chemical process industry. Among the separation processes, distillation is perhaps the most important and energy consuming operation. Hence accurate knowledge of vapour liquid equilibrium (VLE) of the system is of utmost importance for the optimum design and efficient operation of a distillation column. Phenol is a very useful physical solvent. A literature search reveals that there is very little information on vapour liquid equilibria (VLE) of phenol–alcohol systems. The only literature information[1] is not easily available. In an attempt to fill the gap, recently Veeranna and coworkers[2,3] published experimental data and the model parameters for binary systems of phenol with *i*-propanol, *i*-butanol and *n*-butanol. In this work bubble temperature data and the model parameters are presented for the binary system phenol-*n*-propanol.

Isobaric data as compared to isothermal data is of more practical value in process engineering calculations. Hence the experiments were carried out at three constant pressures: 200 mm Hg, 400 mm Hg and 710 mm Hg.

EXPERIMENTAL SECTION

The vapour–liquid equilibrium measurements were conducted in a Swietoslawski ebulliometer[4]. The ebulliometer was connected to a vacuum system. The pressures were measured by a mercury manometer with an accuracy of ±1 mm Hg. The temperature was measured with a PT100 thermometer with an accuracy of 0.1°C.

The boiling points of the system phenol-*n*-propanol were determined over the entire composition range at 200, 400 and 710 mm Hg. Mixtures of different compositions were prepared gravimetrically. The boiling point was first determined at 200 mm Hg. The temperature was recorded when it remained constant for about half an hour. Then the pressure is raised to 400 mm Hg and 710 mm Hg and the procedure is repeated.

PURITY OF THE MATERIALS

Purified *n*-propanol, which has minimum guaranteed purity of 99.0% (assay GC), was obtained from Thomas Bakers Ltd., London. Pure phenol with a minimum guaranteed purity of 99.5% (assay GC) was supplied by Loba Chemie Ltd (India).

These chemicals were used without any further purification. However, the purity of these materials is checked by measuring the physical properties. The comparison of measured physical properties with literature values is shown in Table 1. The measured values are in good agreement with the literature values[5].

RESULTS AND DISCUSSION

The experimental $t - x$ measurements at the three different pressures are presented in Tables 2–4. Here the experimental data are correlated by two different approaches: (i) Equation of state (EOS) approach with the Soave modification of Redlich–Kwong equation and (ii) Gamma–Phi method with Wilson, NRTL and UNIQUAC equations.

Equation of state approach

The details of the Soave equation used in this work may be obtained from the works of Graboski *et al.*[6] or from our earlier work[2]. The bubble-point calculations were carried out by using the algorithm proposed by Veeranna and Rihani[7]. An optimum binary interaction parameter k_{ij} of -0.043 obtained by minimising absolute deviation

Table 1 Comparison of physical properties of pure components with literature values.

	n-Propanol		*Phenol*	
	Measured	*Lit*[5]	*Measured*	*Lit*[5]
Refractive index	1.3855	1.3854 @ 20°C	1.538	1.54 @ 45°C
Boiling point, °C	97.8	97.8	181.6	181.8
Melting point °C			40.9	40.9

Table 2 VLE data for phenol-n-propanol system at 200 mm Hg.

x_1, *mol. fr.*	t_{exp} °*C*	*Soave equation*		*Wilson equation*		*NRTL equation*		*UNIQUAC equation*	
		t_{cal}, °*C*	y_1,cal	t_{cal}, °*C*	y_1,cal	t_{cal}, °*C*	y_1,cal	t_{cal}, °*C*	y_1,cal
0.1120	67.9	67.6	0.0029	68.2	0.0027	68.2	0.0028	68.1	0.0026
0.1989	70.4	70.2	0.0063	70.7	0.0061	70.6	0.0061	70.6	0.0059
0.3341	76.8	75.0	0.0156	75.4	0.0150	75.3	0.0149	75.4	0.0147
0.4113	78.7	78.4	0.0245	78.7	0.0234	78.6	0.0232	78.7	0.0231
0.4432	79.9	80.0	0.0292	80.2	0.0279	80.0	0.0276	80.2	0.0277
0.5645	88.4	86.8	0.0558	86.8	0.0538	86.6	0.0532	87.0	0.0541
0.6450	92.8	92.3	0.0867	92.2	0.0835	92.0	0.0827	92.4	0.0846
0.7313	97.4	99.3	0.1403	99.2	0.1365	99.1	0.1357	99.5	0.1392
0.8022	105.2	106.4	0.2142	106.3	0.2109	106.2	0.2104	106.6	0.2156
0.8990	119.0	119.1	0.4117	119.0	0.4139	119.0	0.4141	119.3	0.4209
0.9378	126.0	125.8	0.5602	125.6	0.5644	125.6	0.5648	125.8	0.5709

Table 3 VLE data for phenol-n-propanol system at 400 mm Hg.

x_1, *mol. fr.*	t_{exp} °*C*	*Soave equation*		*Wilson equation*		*NRTL equation*		*UNIQUAC equation*	
		t_{cal}, °*C*	y_1,cal	t_{cal}, °*C*	y_1,cal	t_{cal}, °*C*	y_1,cal	t_{cal}, °*C*	y_1,cal
0.1120	83.3	83.7	0.0036	84.0	0.0034	84.0	0.0035	83.9	0.0033
0.1989	86.0	86.5	0.0079	86.8	0.0076	86.7	0.0077	86.6	0.0074
0.3341	92.1	91.9	0.0193	92.0	0.0185	91.9	0.0184	91.9	0.0182
0.4113	94.5	95.6	0.0296	95.6	0.0286	95.5	0.0284	95.6	0.0283
0.4432	97.3	97.3	0.0352	97.3	0.0340	97.1	0.0337	97.3	0.0337
0.5645	104.9	104.6	0.0662	104.5	0.0642	104.4	0.0637	104.6	0.0646
0.6450	109.8	110.6	0.1004	110.4	0.0981	110.3	0.0975	110.6	0.0993
0.7313	118.9	118.2	0.1593	118.0	0.1573	117.9	0.1568	118.3	0.1598
0.8022	124.9	125.8	0.2385	125.6	0.2382	125.6	0.2379	125.9	0.2419
0.8990	139.0	139.3	0.4440	139.2	0.4483	139.2	0.4483	139.3	0.4528
0.9378	146.2	146.3	0.5901	146.1	0.5965	146.1	0.5966	146.1	0.6002

Table 4 VLE data for phenol-n-propanol system at 710 mm Hg.

x_1, *mol. fr.*	t_{exp} °C	*Soave equation*		*Wilson equation*		*NRTL equation*		*UNIQUAC equation*	
		t_{cal}, °C	y_1,cal	t_{cal}, °C	y_1,cal	t_{cal}, °C	y_1,cal	t_{cal}, °C	y_1,cal
0.1120	98.0	98.6	0.0044	98.6	0.0041	98.6	0.0042	98.5	0.0040
0.1989	100.1	101.7	0.0097	101.6	0.0091	101.6	0.0091	101.5	0.0088
0.3341	109.3	107.5	0.0230	107.3	0.0218	107.3	0.0217	107.3	0.0215
0.4113	109.5	111.5	0.0350	111.3	0.0333	111.2	0.0332	111.3	0.0331
0.4432	113.1	113.3	0.0414	113.1	0.0394	112.9	0.0392	113.1	0.0393
0.5645	121.8	121.2	0.0762	120.9	0.0735	120.8	0.0731	121.0	0.0739
0.6450	126.8	127.6	0.1141	127.3	0.1109	127.2	0.1105	127.4	0.1120
0.7313	134.3	135.7	0.1780	135.5	0.1751	135.4	0.1748	135.6	0.1772
0.8022	144.8	143.8	0.2621	143.7	0.2607	143.7	0.2605	143.8	0.2635
0.8990	158.0	158.1	0.4726	158.0	0.4747	158.0	0.4748	158.0	0.4774
0.9378	165.8	165.3	0.6169	165.2	0.6202	165.2	0.6204	165.1	0.6221

Table 5 Model parameters for Wilson, NRTL and UNIQUAC equations.

Model	*Parameters*	*RMS error in temperature*
Wilson	$\Delta\lambda_{12} = -15.6769$ K $\Delta\lambda_{21} = -142.253$ K	0.9 K
NRTL ($\alpha_{12} = 0.12$)	$\Delta g_{12} = -97.4770$ K $\Delta g_{21} = -67.1547$ K	0.9 K
UNIQUAC	$\Delta U_{12} = -52.1272$ K $\Delta U_{21} = -39.1916$ K	1.0 K

of experimental and calculated temperatures gave an average absolute deviation of 0.6°C. The observed and calculated temperatures and vapour compositions are also presented in Tables 2–4.

Gamma-phi approach

In this approach the experimental data were correlated with the models: Wilson[8], NRTL[9] and UNIQUAC[10]. The details of these models can be obtained from the above references or from the earlier work[2]. In all the three cases, the gas phase is assumed to be ideal and hence the fugacity coefficient is taken as 1.0. The optimum model parameters in each case were obtained by minimising sum of the squares of the deviation in bubble pressure, using Nelder–Mead optimisation technique. The model parameters along with root mean square error in temperature are presented in Table 5.

All the Gamma–Phi methods correlated the data with same accuracy. Surprisingly, the Soave equation correlated the data very well with devation comparable to the Gamma–Phi methods. The calculated temperatures and vapour compositions for all the three models are presented in Table 2–4. As can be seen from these tables, the predictions from all the models are almost same.

CONCLUSIONS

The system is well correlated by all the models studied here. The assumption of ideal vapour phase behaviour is justified because the pressures treated here are low. The Soave equation correlated the data remarkably well even with temperature independent binary interaction parameter. The correlation by Soave equation is as good as that by Gamma–Phi methods. Hence it can be expected that Soave equation would correlate well other phenol–alcohol systems also.

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