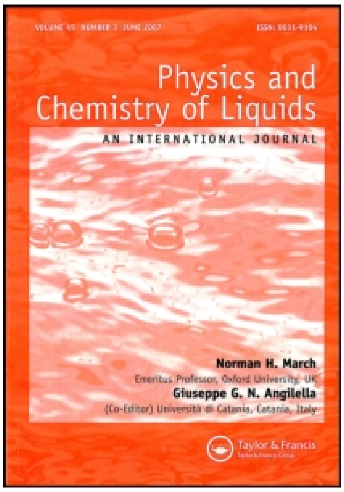

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ISOBARIC VAPOUR LIQUID EQUILIBRIUM DATA FOR BINARY SYSTEMS PHENOL-DI-ISOPROPYL ETHER AND 2,4-XYLENOL-DI-ISOPROPYL ETHER

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Motivated by chemical engineering design purposes, isobaric vapour liquid equilibrium data on two binary mixtures has been obtained. The temperature-mole fraction data were measured in a Swietoslawski ebulliometer.

KEY WORDS: Vapour pressures and compositions, binary mixtures.

INTRODUCTION

For the economic viability of the low temperature carbonization of coal it is necessary to process the resulting tar to yield the value-based chemicals such as phenols. During the processing of tar, the di-isopropyl ether-phenol mixtures are encountered, necessitating the use of vapor liquid equilibrium (vle) data on such systems for designing separation plants. The aim of the present work is to report the results obtained on the vle studies on the Phenol-Di-iso propyl ether and 2,4-Xylenol-Di-isopropyl ether binary mixtures, at an isobaric pressure of 723 mm Hg. The vapor compositions, y, corresponding to the measured temperature (t)-mole fraction (x) data are computed by using the NRTL method.

EXPERIMENTAL SECTION

The t-x measurements on the two binaries were carried out in a Swietoslawski ebulliometric set up described briefly elsewhere[1]. The materials used in the investigation were purified by means of a Podbielniak hypercal distillation column. The physical properties of the materials are reported in Table 1 along with those from the literature

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used for comparison purposes. The Antoine constants needed for the calculation of the pure component vapor pressures are also reported in the Table. The pressure and the temperature measurements reported in the present work were precise to 1 mm Hg and 0.1°C respectively.

About 130 ml. of the binary mixture was introduced into the ebulliometer. A steady reading on the mercury thermometer accompanied by a steady condensate drop rate (using the drop counter) in the range of 20–30 drops per minute as recommended by Hala *et al*[2], were taken as the criteria for the attainment of the equilibrium between the phases.

RESULTS AND DISCUSSION

The vapor composition of the component i (y_i) is calculated from the equation

$$P_t Y_i \varphi_i = \gamma_i P_i^0 X_i \tag{1}$$

where P_t and P_i^0 are total pressure of system, vapor pressure of the component i, φ and γ are the vapor phase non-ideality factor and the activity coefficient respectively and x_i and y_i are the mole fractions of the component i in liquid and vapor phases respectively. For near-ideal vapor phase condition, where in $\varphi_i \simeq 1.0$ the Eqn. (1) reduces to the form

$$P_t Y_i = \gamma_i P_i^0 X_i \tag{2}$$

For a binary system one can write:

$$P_t = X_1 P_1^0 \gamma_1 + X_2 P_2^0 \gamma_2 \tag{3}$$

Table 1 Densities, refractive indices and Antoine constants of pure compounds.

Compound	*Density, g·ml⁻¹*			*Ref. Index*		
	This work	*Lit.*	*Ref.*	*This work*	*Lit.*	*Ref.*
Phenol	1.0537(45)*	1.0540	6	1.5415(41)	1.5417	4
2,4-Xylenol	1.0165(25)	1.0160	7	1.5417(20)	1.5420	5
Di-isopropyl ether	0.7209(23)	0.7200	6	1.3690(23)	1.3678	6

Antoine Constants

Compound	*A*	*B*	*C*	*Ref.*
Phenol	7.13457	1516.07	174.569	7
2,4 Xylenol	7.04694	1581.40	168.650	7
Di-isopropyl ether	6.93051	1172.45	221.220	5

*Values given in brackets denote the reference temperature in °C.

The vapor pressures P_1^0 and P_2^0 are calculated by using the Antoine equation

$$\log P^0 = A - \frac{B}{t + C} \tag{4}$$

where P^0 is in mm Hg, corresponding to the temperature in °C. The activity coefficients γ_1 and γ_2 are calculated by means of the well-known NRTL model[3], where the model parameters $(g_{12} - g_{22})$, $(g_{22} - g_{11})$ and a_{12} are assumed to be the functions of temperature represented by the equations:

$$\begin{aligned} g_{12} - g_{22} &= A_1 + B_1(T - 273.15) \\ g_{22} - g_{11} &= A_2 + B_2(T - 273.15) \\ a_{12} &= A_3 + B_3(T - 273.15) \end{aligned} \tag{5}$$

with T in °K and $A_1, A_2 \ldots B_1 \ldots B_3$ as the constants.

Substituting the values of the activity coefficients γ_1 and γ_2 calculated from the NRTL equation and the vapor pressures of the pure components, P_1^0 and P_2^0 (calculated from the Eqn. (4)) in the equation

$$P_{t,\mathrm{cal}} = X_1 P_1^0 \gamma_1 + X_2 P_2^0 \gamma_2 \tag{6}$$

the total pressure P_t is calculated.

Table 2 lists the values of the NRTL constants $A_1 \ldots B_3$ needed for the calculation of the activity coefficients along with the % average absolute deviations ($\bar{e}$) obtained for the two binaries studied.

The % average absolute deviation $\bar{e}$, is calculated from

$$\bar{e} = \frac{E\,|e|}{N} \tag{7}$$

Table 2 Temperature-dependent NRTL Model Parameters and Percent Average Absolute Deviations (PAAD) on Pressure.

System	*Parameters (Eq. 5)*		*No. of data points*	*Temperature Range, °C*	*PAAD*
Phenol (1)-Di-isopropyl ether (2)	$A1 = 1398$ $A2 = 9159$ $A3 = 0.1149$	$B1 = -9.011$ $B2 = -15.94$ $B3 = 0.001332$	17	65.9 – 167.4	2.9
2,4 Xylenol(1)-Di-isopropyl ether (2)	$A1 = 205.03$ $A2 = 1243.00$ $A3 = -0.02557$	$B1 = 1.4693$ $B2 = -7.6501$ $B3 = 0.006541$	17	67.8 – 179.1	1.6

Table 3 VLE Data for the Systems Phenol(1)-Di-isopropyl ether (2) and 2,4-Xyleneol(1)-Di-isopropyl ether (2) at 723 mm Hg.

t,°C	*Phenol(1)-Di-Isopropyl ether (2)*		*PAAD on Pressure*
	x_1	y_1^*	
65.9	0.0562	0.0027	7.0
67.1	0.1094	0.0039	7.9
68.1	0.1970	0.0060	4.3
68.5	0.2694	0.0076	0.5
69.1	0.3130	0.0084	−0.7
69.8	0.3634	0.0093	−1.5
71.2	0.4156	0.0103	0.0
71.9	0.5180	0.0115	−2.7
79.1	0.7103	0.0161	6.1
82.1	0.7913	0.0198	2.8
87.9	0.8453	0.0283	−1.0
94.4	0.8630	0.0388	0.0
112.4	0.8850	0.0834	6.1
119.4	0.9028	0.1199	0.0
135.3	0.9200	0.2228	0.0
145.3	0.9357	0.3347	−3.8
167.4	0.9618	0.6375	4.7
% average absolute deviation			2.9

t,°C	*2,4-Xylenol(1)-Di-isopropyl ether (2)*		*PAAD on Pressure*
	x_1	y_1^*	
67.8	0.0862	0.0020	−2.0
68.4	0.1690	0.0023	−2.1
68.8	0.2158	0.0024	−1.3
69.4	0.2919	0.0025	0.0
70.6	0.3934	0.0026	2.3
70.9	0.4979	0.0028	0.8
71.9	0.6022	0.0032	−1.5
77.2	0.7025	0.0045	0.6
82.6	0.8006	0.0071	−6.3
94.8	0.8502	0.0132	2.0
96.9	0.8695	0.0156	−2.4
104.9	0.8927	0.0231	0.4
106.9	0.9019	0.0263	−1.6
113.3	0.9184	0.0362	−2.5
122.6	0.9316	0.0531	1.4
146.1	0.9595	0.1406	0.0
179.1	0.9755	0.4268	0.0
% average absolute deviation			1.6

y_1^* calculated from NRTL model.

where E is the summation of the modulus of the errors, e, determined over N data points. The error e is estimated from

$$e = 100\left(\frac{P_{t,\,\mathrm{exp}} - P_{t,\,\mathrm{Calc}}}{P_{t,\,\mathrm{exp}}}\right) \tag{8}$$

where $P_{t,\mathrm{exp}}$ is the isobaric experimental pressure over which the data were obtained. In the present work, the t-x data were obtained at a pressure of 723 mm Hg.

The results obtained on fitting vapor compositions, y, to the t-x data (obtained from the ebulliometer), using the method described are reported in Table 3. It can be seen from the Tables 2 and 3 that the data are adequately represented by the NRTL method and hence can be used for design purposes.

NOMENCLATURE

A, B, C	Antoine Constants
A_1, A_2, A_3	NRTL temperature-dependent parameters defined by the Eqn. (5)
B_1, B_2, B_3	
e	percent deviation between the experimental and calculated pressures defined by the Eqn. (8).
g	interaction parameter in the NRTL equation
i	component
N	number of data points
P_t	total pressure, mm Hg
P^0	vapor pressure, mm Hg
T	absolute temperature, °K
t	temperature in °C
X	liquid phase mole fraction
Y	vapor phase mole fraction
$\|\|$	modulus
E	summation of
a	Non-randomness parameter in the NRTL equation
γ	activity coefficient
φ	vapor phase non-ideality factor

Subscripts

exp	experimental value of
cal	calculated value of

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