

Vapor–Liquid Equilibrium in α -Methylbenzenemethanol + Water

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The saturation pressure of α -methylbenzenemethanol at (293 to 363) K was measured by the static method. The total pressure (P , T , x) was measured by the static method for the system α -methylbenzenemethanol + water at (293.15, 303.15, 313.15, 323.15, 333.15, 343.15, 353.15, and 363.15) K. The system is forming two liquid phases. The solubility was determined with the ampule method. The density inversion temperature was observed in the liquid phases. An azeotrope was found in the system. Below 350 K, it is a positive homoazeotrope, while above this temperature it is a positive heteroazeotrope. The experimental vapor pressures were correlated with the Antoine equation, while VLE was correlated with the NRTL equation.

Introduction

α -Methylbenzenemethanol is used as a flavoring agent in foods and beverages; it also occurs naturally in a variety of foods. On the other hand, it may be harmful if swallowed or inhaled. Its carcinogenic properties are also investigated.¹ Due to this, properties of its mixtures with water are interesting. The VLE data for the system α -methylbenzenemethanol + water have not been reported in the literature, and the results cannot be predicted with sufficient accuracy either by using pure component property data or using a semiempirical method (e.g., based on a group contribution concept such as ASOG² or UNIFAC³).

Experimental Section

Chemicals. α -Methylbenzenemethanol (Chemical Abstracts Service Registry No. (CASRN) 98-85-1) purchased from Fluka (purity > 98 %) was distilled at subambient pressure ($p/\text{kPa} = 4$) on a 30 theoretical plate column. The purity of fractions was checked by GLC (with FID detector) on the FFAP 30 m long capillary column, and those of purity better than 99.8 mol % were collected and used. The water content detected by GLC was lower than 0.001 mol %. Water (CASRN 7732-18-5) was distilled three times from alkali potassium permanganate solution. The distillate was acidified with sulfuric acid and distilled twice. The final distillation was put into a degassing vessel (Figure 3). Degassing has been made in the vessel connected through valve K_7 to the vacuum line (Figure 1) by distilling water from one arm of the vessel to another. After each distillation, the vessel has been degassed through the K_7 valve. This procedure was repeated seven times. Mercury (CASRN 7439-97-6) supplied by POCh–Gliwice was purified after each series of measurements by washing with 8 mass % nitric acid and distilled water, dried in acetone, and finally distilled under reduced pressure.

Analytical Procedure. For initial determination of the purity of α -methylbenzenemethanol, the GLC method with the HP 5890 series II gas chromatograph equipped with an HP 3396 integrator, a thermal conductivity detector (TCD), and a HP-FFAP (poly(ethylene glycol)-TPA modified) 30 m \times 0.53 mm \times 0.01 μm film thickness column was used. An internal standard was used in the calibration procedure.

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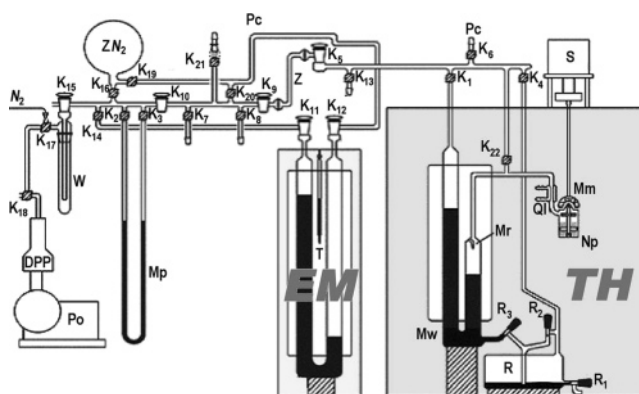


Figure 1. Static apparatus for determination of the vapor–liquid equilibria in systems forming two liquid phases: EM, external mercury manometer; TH, liquid thermostat; DPP, vacuum diffusion pump; K_1 to K_{22} , glass valves; Mm, rotating magnet; Mr, cell constant volume marker; Mp, control manometer; Ms, spinning magnet; Mw, internal manometer; N_2 , nitrogen inlet; Np, equilibrium cell; Pc, connection to McLeod-type vacuum gauge; Po, rotary vacuum pump; Ql, cooler; R, internal manometer mercury reservoir; R_1 to R_3 , glass valves with Teflon rods for manipulation of mercury level; S, magnetic stirrer motor; T, mercury thermometer; W, cold trap; Z, flexible connection with spherical joints; ZN_2 , nitrogen container.

VLE Apparatus. The previously described⁴ static VLE apparatus especially designed for the measurements of systems forming one or more liquid phases was used. The schematic diagram of the apparatus is given in Figure 1. The glass apparatus consists of a high vacuum line and a measuring section, immersed in a water thermostat enabling visual observation of the equilibrium cell (Np) and the internal mercury manometer (Mw). The details of thermostat construction were described earlier.⁵ The internal manometer is working as a null indicator. Prior to measurements, the total volume of the equilibrium cell (Np), including all connecting tubing up to the marker (Mr) in the internal manometer, should be determined.

Vacuum was obtained by means of a rotary pump (Po) coupled with a diffusion pump (DPP) and checked with a precision of ± 0.1 Pa by a portable McLeod gauge, connected to valves K_{21} or K_6 . The vacuum line consists of the ampule preparation section (between valves K_9 and K_{10}), a nitrogen container (ZN_2) section, and a pressure maintaining section between the internal and external manometers. The manometer (Mp) controls pressure in the line to prevent over-pressurization

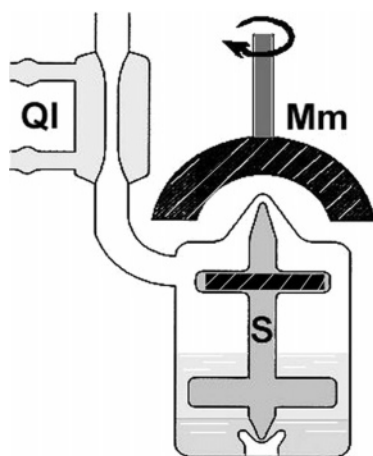


Figure 2. Equilibrium cell: Ql, cooler; S, magnetic stirrer; Mm, rotating magnet.

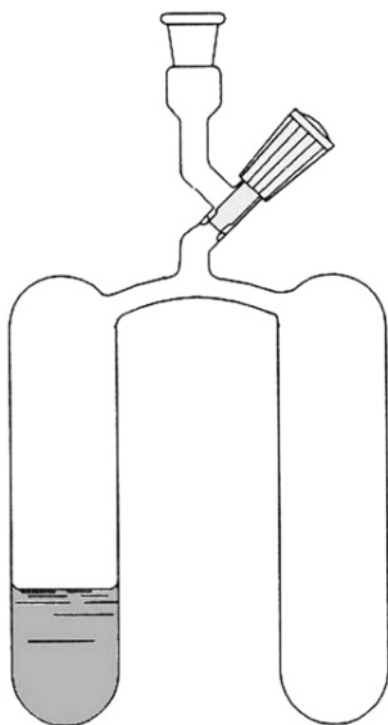


Figure 3. Degassing vessel.

during maintenance of the system with gaseous nitrogen introduced through valve K_{17} . The equilibrium cell (Np) equipped with a magnetic stirrer (S) is shown in detail in Figure 2.

The equilibrium pressure was determined by two thermostated mercury manometers, internal and external, with one located in an air thermostat. The level of mercury was measured by means of a cathetometer with accuracy of ± 0.005 mm. The equilibrium temperature was measured with a Systemtechnik AB S1228 thermometer with a 100Ω platinum resistance probe (resolution, 0.001 K). The calibration was made by comparison with readings of a Tinsley & Co Muller Bridge type 4772 with a platinum resistance temperature sensor type 5187 SA calibrated by NPL to type I (uncertainty ± 0.001 K). The temperature fluctuation during runs, each lasting several hours, was within ± 0.005 K. No systematic deviations of the temperature were observed. The estimated error was not greater than ± 0.01 K. The temperatures have been converted to the International Temperature Scale of 1990 (ITS-90) according to method described by Preston-Thomas.⁶

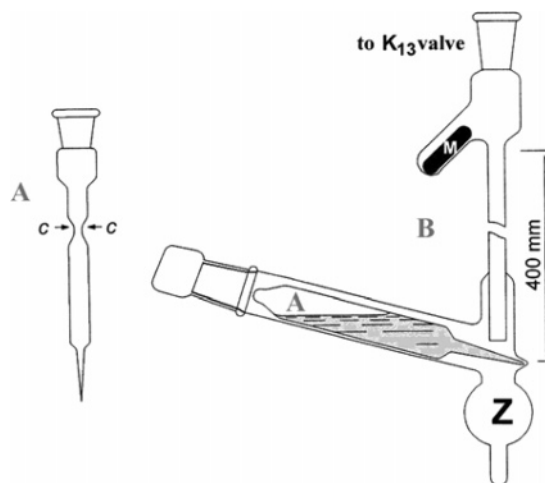


Figure 4. A, sample vial, c-c, soldering line; B, assembly for introducing samples of water to the apparatus; M, Teflon-covered magnet for breaking vial.

Table 1. Vapor Pressure of α -Methylbenzenemethanol and Estimated Standard Uncertainty of Measurements (δP and δT)

T/K	p/Pa	$\delta P/\text{Pa}$	T/K	p/Pa	$\delta P/\text{Pa}$
293.33	9.952	1.6	333.39	263.5	6.0
293.34	9.956	1.6	333.39	264.9	6.0
303.35	24.51	2.0	343.42	515.0	6.0
303.35	21.90	2.0	343.42	518.9	6.0
313.37	62.81	2.0	353.43	902.0	6.0
313.37	64.14	2.0	353.43	905.3	6.0
323.39	147.2	5.0	363.43	1556	6.0
323.39	136.0	5.0	363.43	1556	6.0
323.39	141.9	5.0			

$\delta T/K = 0.01$

Due to low vapor pressure of the alcohol, it was impossible to distill degassed samples directly to the apparatus. The sample of known mass (about 14 g) of alcohol, after introductory degassing, was introduced directly to the equilibrium cell (Figure 2). The cell was soldered to the apparatus, and the sample was degassed within the apparatus in three cycles. The loss of mass during each cycle was negligible (about 0.3 mg to 20 ppm of the sample). The degassing was repeated until no changes in vapor pressure were observed. The samples of water (mass varying from 0.3 g to 8 g) were degassed in the vessel shown in Figure 3 by distilling from one arm of the vessel to the second arm. The procedure was repeated, and finally the sample was distilled into the glass vial shown in Figure 4 (A) and sealed under vacuum.

Vapor Pressure. The vapor pressure measurements of the degassed sample of α -methylbenzenemethanol were made in the described VLE apparatus. The measurement starts at the lowest temperature. The readings were taken after the temperature was stable within ± 2 mK for 30 min. Then the temperature was raised; and after about 90 min, once more when the stability was ± 2 mK, the readings were taken. During each vapor pressure measurement, the mercury levels in internal manometer should be fixed at Mr marker and identical in both arms. This is achieved by moving mercury to and from the R container. This procedure enables the maintenance of constant volume of the equilibrium cell. The procedure was repeated three times for each temperature. The results obtained are given in Table 1.

Vapor-Liquid Equilibrium. The VLE was determined by the total pressure method, that is, by determination of the pressure in the equilibrium cell at constant volume conditions. The measurements start with pure alcohol, already degassed in the apparatus. The purity of alcohol was checked by determi-

Table 2. Vapor–Liquid Equilibrium of α -Methylbenzenemethanol (1) + Water (2)^a

<i>T</i> /K	<i>x</i> _{1exp}	<i>y</i> _{1calc}	<i>P</i> _{exp} /kPa	no. of phases	<i>T</i> /K	<i>x</i> _{1exp}	<i>y</i> _{1calc}	<i>P</i> _{exp} /kPa	no. of phases	<i>T</i> /K	<i>x</i> _{1exp}	<i>y</i> _{1calc}	<i>P</i> _{exp} /kPa	no. of phases
293.15	0.0000	0.0000	2.333	1	313.15	0.6600	0.0048	7.474	2	343.15	0.2626	0.0339	31.248	2
293.15	0.0754	0.0771	2.394	2	313.15	0.7635	0.0054	6.430	1	343.15	0.3297	0.0219	31.371	2
293.15	0.0941	0.0416	2.291	2	313.15	0.8723	0.0086	4.217	1	343.15	0.4247	0.0148	31.400	2
293.15	0.1189	0.0509	2.330	2	313.15	1.0000	1.0000	0.041	1	343.15	0.4369	0.0140	31.140	2
293.15	0.1594	0.0336	2.343	2	323.15	0.0000	0.0000	12.338	1	343.15	0.5807	0.0115	31.152	2
293.15	0.1998	0.0174	2.356	2	323.15	0.0754	0.0789	12.491	2	343.15	0.6643	0.0115	29.698	1
293.15	0.2623	0.0071	2.366	2	323.15	0.0941	0.0681	12.299	2	343.15	0.7678	0.0139	24.438	1
293.15	0.3290	0.0042	2.394	2	323.15	0.1189	0.0731	12.409	2	343.15	0.8760	0.0230	15.584	1
293.15	0.4235	0.0026	2.380	2	323.15	0.1594	0.0586	12.372	2	343.15	1.0000	1.0000	0.404	1
293.15	0.4347	0.0027	2.361	2	323.15	0.1997	0.0416	12.375	2	353.15	0.0000	0.0000	47.382	1
293.15	0.5769	0.0022	2.273	2	323.15	0.2623	0.0225	12.379	2	353.15	0.0754	0.0794	47.524	2
293.15	0.6599	0.0021	2.407	2	323.15	0.3291	0.0138	12.448	2	353.15	0.0942	0.0841	47.557	2
293.15	0.7628	0.0023	2.187	2	323.15	0.4237	0.0091	12.450	2	353.15	0.1190	0.0866	47.658	2
293.15	0.8722	0.0036	1.447	1	323.15	0.4352	0.0087	12.345	2	353.15	0.1596	0.0797	47.728	2
293.15	1.0000	1.0000	0.006	1	323.15	0.5083	0.0075	12.316	2	353.15	0.2001	0.0628	47.552	2
303.15	0.0000	0.0000	4.240	1	323.15	0.5777	0.0070	12.339	2	353.15	0.2629	0.0400	47.547	2
303.15	0.0754	0.0779	4.329	2	323.15	0.6609	0.0067	12.290	1	353.15	0.3302	0.0265	47.720	2
303.15	0.0941	0.0516	4.190	2	323.15	0.7645	0.0078	10.376	1	353.15	0.4254	0.0182	47.600	2
303.15	0.1189	0.0593	4.250	2	323.15	0.8731	0.0124	6.750	1	353.15	0.4382	0.0171	47.363	2
303.15	0.1594	0.0424	4.253	2	323.15	1.0000	1.0000	0.095	1	353.15	0.5122	0.0151	47.344	2
303.15	0.1997	0.0258	4.267	2	333.15	0.0000	0.0000	19.924	1	353.15	0.5828	0.0141	47.178	2
303.15	0.2622	0.0120	4.278	2	333.15	0.0754	0.0792	20.100	2	353.15	0.6668	0.0145	44.001	1
303.15	0.3289	0.0071	4.307	2	333.15	0.0941	0.0746	19.919	2	353.15	0.7702	0.0177	35.914	1
303.15	0.4234	0.0045	4.306	2	333.15	0.1189	0.0786	20.049	2	353.15	0.8782	0.0297	22.642	1
303.15	0.4346	0.0044	4.269	2	333.15	0.1594	0.0661	19.999	2	353.15	1.0000	1.0000	0.759	1
303.15	0.5074	0.0038	4.241	2	333.15	0.1998	0.0490	19.975	2	363.15	0.0000	0.0000	70.180	1
303.15	0.5767	0.0035	4.187	2	333.15	0.2624	0.0281	19.972	2	363.15	0.0755	0.0793	70.221	2
303.15	0.6597	0.0033	4.349	2	333.15	0.3293	0.0177	20.063	2	363.15	0.0942	0.0872	70.521	2
303.15	0.7629	0.0036	3.833	1	333.15	0.4241	0.0118	20.070	2	363.15	0.1191	0.0892	70.531	2
303.15	0.8720	0.0056	2.528	1	333.15	0.4359	0.0112	19.911	2	363.15	0.1597	0.0859	70.858	2
303.15	1.0000	1.0000	0.016	1	333.15	0.5092	0.0098	19.886	2	363.15	0.2003	0.0691	70.519	2
313.15	0.0000	0.0000	7.376	1	333.15	0.5790	0.0091	19.946	2	363.15	0.2633	0.0463	70.536	2
313.15	0.0754	0.0785	7.497	2	333.15	0.6623	0.0089	19.437	1	363.15	0.3307	0.0313	70.790	2
313.15	0.0941	0.0604	7.324	2	333.15	0.7659	0.0106	16.172	1	363.15	0.4263	0.0218	70.600	2
313.15	0.1189	0.0667	7.409	2	333.15	0.8743	0.0173	10.423	1	363.15	0.4397	0.0204	70.233	2
313.15	0.1594	0.0507	7.394	2	333.15	1.0000	1.0000	0.203	1	363.15	0.5142	0.0181	70.197	2
313.15	0.1997	0.0339	7.407	2	343.15	0.0000	0.0000	31.169	1	363.15	0.5855	0.0170	69.496	1
313.15	0.2622	0.0171	7.416	2	343.15	0.0754	0.0794	31.347	2	363.15	0.6698	0.0178	63.420	1
313.15	0.3290	0.0103	7.468	2	343.15	0.0941	0.0799	31.232	2	363.15	0.7730	0.0220	51.469	1
313.15	0.4235	0.0067	7.460	2	343.15	0.1190	0.0831	31.365	2	363.15	0.8809	0.0374	32.061	1
313.15	0.4347	0.0064	7.398	2	343.15	0.1595	0.0731	31.334	2	363.15	1.0000	1.0000	1.352	1
313.15	0.5770	0.0051	7.345	2	343.15	0.1999	0.0561	31.256	2					
Azeotropic Parameters ^b														
293.15	0.0022	0.0022	2.353	1	323.15	0.004	0.004	12.387	1	353.15	0.008	0.008	47.572	2
303.15	0.0028	0.0028	4.270	1	333.15	0.005	0.005	19.998	1	363.15	0.008	0.008	70.589	2
313.15	0.0032	0.0032	7.414	1	343.15	0.006	0.006	31.286	1					

^a Standard uncertainties: $\delta(T)/K = 0.01$; $\delta(x_1) = 0.0003$; $\delta(y_1) = 0.001$; $\delta(P)/Pa = 3$. ^b Experimental standard uncertainties: $\delta(T)/K = 0.01$; $\delta(x_1) = 0.01$; $\delta(P)/Pa = 3$.

nation of vapor pressure in the range from 293 K to 363 K. To obtain mixtures, the sealed samples of known mass of water, determined by weighing, were introduced to the equilibrium cell (Np) through the assembly shown in Figure 4 and connected to the apparatus through valve K₁₃. The glass vials were broken with a magnetic rod, and the sample was distilled into the apparatus. During distillation, the equilibrium cell was frozen, and mercury from the internal manometer was transferred to container R. The estimated accuracy of a binary sample composition was ± 0.03 wt %. The vapor pressure measurements start at the lowest temperature after the desired stability of temperature is achieved. Then the temperature is raised to the next value. While temperature is increasing, the outlet of equilibrium cell is cooled with cooler Q1 to prevent condensation of sample components in the internal manometer. After pressure was determined for all assumed temperatures, the next sample of water was introduced to the apparatus, and pressure measurements were repeated for a new composition. The azeotropic parameters were determined by the analysis of the

shape of each dew points isotherm. The results obtained are given in Table 2.

Liquid–Liquid Equilibrium. The mutual solubility was determined with the ampule method.⁷ Both substances were injected into the glass ampule. To enable good mixing, a glass ball of diameter slightly smaller than the ampule bore was introduced to the ampule. Masses of added liquids were determined by weighting with an uncertainty of ± 0.0003 g. The volume of the sample was 5 cm³, and consequently, the uncertainty of mole fraction was better than 10⁻⁴. The ampule was cooled with solid carbon dioxide and sealed by welding. The ampules with samples were immersed in an earlier described thermostat.⁷ The temperature in the thermostat was measured with Systemtechnik AB S1228 platinum resistance thermometer with the uncertainty of ± 0.002 K and controlled with a temperature controller (type 650 with power unit type 651, Nipan, Poland) to ± 0.002 K. During the experiment, the samples were continuously mixed by rocking the ampule. The equilibrium temperature was determined visually either by the

Table 3. Liquid–Liquid Equilibrium of α -Methylbenzenemethanol (1) + Water (2)^a

x_1	T/K	x_1	T/K
0.0097	365.87	0.5646	368.05
0.4588	401.08	0.7624	293.00
0.5457	379.11	0.7896	287.73

^a Experimental standard uncertainties: $\delta(T)/K = 0.03$; $\delta(x_1) = 0.0001$.

Table 4. Isodensity Temperatures of Coexisting Liquids^a

x_1	T/K
0.008	325
0.104	325
0.459	325

^a Experimental standard uncertainties: $\delta(T)/K = 1$; $\delta(x_1) = 0.003$.

disappearance of a liquid phase or the appearance of opalescence when the cycles of heating and cooling were repeated. The temperature near equilibrium was changed very slowly at a rate of about $0.01 \text{ K}\cdot\text{min}^{-1}$. The results obtained are given in Table 3. The values reported are mean from at least five consecutive measurements for each composition. The precision of the equilibrium composition was better than $\pm 5 \times 10^{-5}$ of mole fraction, uncertainties result from partial evaporation of the lighter component to the free volume of the ampules, which varied from about 0.5 cm^3 to 1.0 cm^3 .

During measurements, an interesting phenomenon was observed. At room temperature the alcohol rich phase has higher density than the in water rich phase. Above 333 K, the water rich phase has higher density. To determine the inversion temperature, the sample of known composition was introduced into the glass ampule and vigorously stirred at constant temperature. After the stirring was stopped, the separation of phases was observed. The temperature when one of phases remains in the highest and lowest layer of the sample, while the second phase remains in the middle layer was considered the inversion temperature. The results obtained are given in Table 4.

Correlation

Vapor pressure data were correlated with the Antoine equation:

$$\log(p/\text{kPa}) = A - \frac{B}{T/K - C} \quad (1)$$

where p is pressure; T is temperature; and A , B , and C are adjustable parameters. Deviations of experimental data from these computed from the Antoine equation are given in Table 1. The root mean square deviations (δ_{rms}) of p are calculated from

$$\delta_{\text{rms}}(p)/\text{Pa} = \sqrt{\frac{\sum_{i=1}^n (p_i^{\text{calcd}} - p_i^{\text{exptl}})^2}{n}} \quad (2)$$

The parameters of the Antoine equation are listed in Table 5 together with the $\delta_{\text{rms}}(p)$. For water, the parameters calculated by NIST⁸ from Bridgeman and Aldrich data⁸ were used. The vapor pressure data were compared with those of Dreisbach and Shrader¹⁰ and earlier investigations from our laboratory.¹¹ The comparison is given in Figure 5. The results are satisfactory.

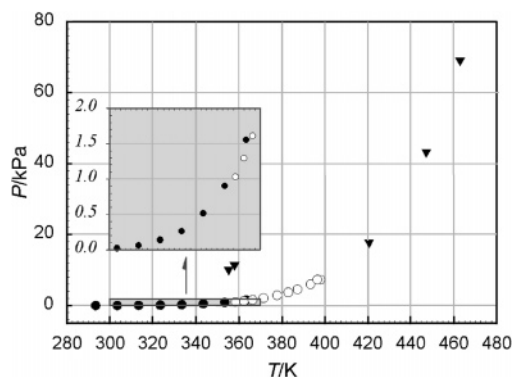


Figure 5. Vapor pressure of α -methylbenzenemethanol: \circ , our measurements; \bullet , ref 5; \blacktriangledown , ref 6.

Table 5. Parameters of the Antoine Equation (eq 1)

substance	temp range	Antoine parameters			$\delta_{\text{rms}}(p)$
	K	A	B	C	Pa
α -methylbenzenemethanol	293–364	6.208042	1614.235	95.126	5.45
water	273–303	7.40221	1838.675	31.737	5.11
	304–333	7.20389	1733.926	39.485	2.61
	334–363	7.07680	1659.793	45.854	44.4

Vapor–Liquid Equilibrium. The volume of the liquid phase in the measuring cell is small in comparison to the volume of the vapor phase. Due to this, a correction for the change of liquid composition due to evaporation should be introduced. The details were given earlier.¹² The computation is made for each isotherm by an iterative method using

$$x_i = q_i \frac{1 + V/L}{1 + y_i V/x_i L} \quad (3)$$

where V and L are amounts of substance in the vapor and liquid phases, respectively; q_i is the mole fraction of component i in the sample introduced to the apparatus; x_i and y_i are the mole fractions of component i in the liquid phase and vapor phases, respectively. The computation starts for $x_i = q_i$ and activity coefficients equal to one. In following iterations, the NRTL equation (eqs 4 and 5) was introduced to represent the relations between x_i and y_i . The iterative procedure is repeated until the difference between values of x_i in consecutive iterations is lower than 10^{-6} . The computed values of vapor composition (y_{calc}) are given in Table 2.

Finally results were fitted to the six-parameter NRTL equation (eqs 4 to 6) using the NRTL program as described by Renon et al.¹³ Only 37 points from one liquid-phase region were used for correlation:

$$g^E(x, T) = RTx_1x_2 \left(\frac{\tau_{21} \exp(-\alpha_{12}\tau_{21})}{x_1 + x_2 \exp(-\alpha_{12}\tau_{21})} + \frac{\tau_{12} \exp(-\alpha_{12}\tau_{12})}{x_2 + x_1 \exp(-\alpha_{12}\tau_{12})} \right) \quad (4)$$

where

$$\tau_{12} = \frac{C_{12}}{RT} \quad \text{and} \quad \tau_{21} = \frac{C_{21}}{RT} \quad (5)$$

The temperature dependence of parameters is given by

$$C_{ji} = C_{ji}^{(0)} + C_{ji}^{(T)}(T - 273.15) \quad \text{and} \quad \alpha_{12} = \alpha_{12}^{(0)} + \alpha_{12}^{(T)}(T - 273.15) \quad (6)$$

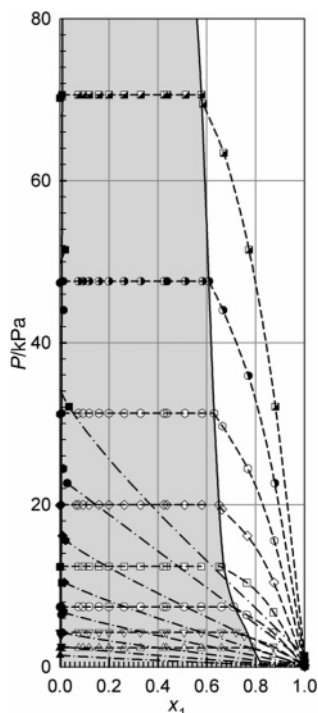


Figure 6. VLE for α -methylbenzenemethanol (1) + water (2): Δ , 293.15 K; ∇ , 303.15 K; \circ , 313.15 K; \square , 323.15 K; \diamond , 333.15 K; \circ , 343.15 K; \bullet , 353.15 K; \blacksquare , 363.15 K. Open symbols represent experimental bubble points, and solid symbols represent dew points. Correlation with the NRTL equation: $- -$, bubble point line, $- \cdot -$, dew point line; gray shading, two liquid-phase region.

Table 6. Parameters of the NRTL Equation (eqs 4 to 6)

$C_{21}^{(0)}$	$C_{12}^{(0)}$	$\alpha^{(0)}$	$C_{21}^{(T)}$	$C_{12}^{(T)}$	$\alpha^{(T)}$	RMSD(x_1)	RMSD(p)/Pa
8786.3	-84.083	0.16993	15.063	3.9127	0.0010528	0.011	279

The rmsd of pressure (rmsd(p)/Pa) and vapor composition (rmsd(y)) were calculated for all experimental points, both from one liquid-phase region and from two liquid-phase regions by

$$\text{rmsd}(p/\text{Pa}) = \sqrt{\frac{\sum_{i=1}^n (p_i^{\text{exp}} - p_i^{\text{calc}})^2}{n - m}}$$

$$\text{rmsd}(y_1) = \sqrt{\frac{\sum_{i=1}^n (y_{1,i}^{\text{exp}} - y_{1,i}^{\text{calc}})^2}{n - m}} \quad (7)$$

where $m = 6$ is the number of adjustable parameters, $n = 128$ is the number of experimental points, p_i^{exp} is the pressure

measured at point number i , and p_i^{calc} is the pressure calculated from NRTL equation at point number i . $y_{1,i}^{\text{exp}}$ is the mole fraction of component 1, calculated by iterative procedure for each particular isotherm measured at point number i , and $y_{1,i}^{\text{calc}}$ is the pressure calculated from the six-parameter polythermal NRTL equation (eqs 4–6) at point number i . The correlation results are summarized in Table 6 and presented in Figure 6.

Conclusions

The VLE in the α -methylbenzenemethanol + water system was measured for the first time. The binary positive homoazeotrope was found at temperatures below 350 K, while above this temperature a positive heteroazeotrope was observed. The experimental data were correlated by means of the NRTL equation.

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