



Original articles

Research article

<https://doi.org/10.17308/kcmf.2022.24/9268>**Liquid-vapour phase equilibria of three-component systems formed by *n*-propanol, *n*-butanol, and *n*-alkylethanoates**Yu. K. Suntsov¹ ✉, G. Yu. Kharchenko², N. S. Suntsova¹¹Voronezh State University,
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86 ul. Lenina, Voronezh, 394043, Russian Federation**Abstract**

The production of *n*-alcohols and ethanoic acid esters involves solving problems regarding the rectification of solutions of multicomponent systems. The main achievements related to the methods of calculating the phase equilibria in multicomponent systems have been associated with the development of equations based on local compositions. Equilibrium in multicomponent systems is predicted using data about the binary components of these systems. The most common local composition models are the Wilson and NRTL equations. Liquid-vapour equilibria of binary systems formed by aliphatic alcohols and esters of organic acids have been already studied. Liquid-vapour equilibria of the studied binary systems have been described by the Wilson and NRTL equations.

Boiling points (the pressure of saturated vapour) of solutions of three-component systems formed by *n*-propanol, *n*-butanol, *n*-propylethanoate, and *n*-butylethanoate were measured under various pressure values using the ebulliometric method. The activity coefficients of the solution components of the three-component systems were calculated using the Wilson and NRTL equations. The parameter values in the Wilson and NRTL equations for the binary systems were calculated by nonlinear regression methods. The results of the calculations were verified experimentally.

It was found that the values of the activity coefficient of *n*-propanol and *n*-butanol increase with a decrease in their concentrations in the solutions of the systems. Similar changes in the values of the activity coefficients of the components in the solutions of the systems were observed for the molecules of *n*-propylethanoate and *n*-butylethanoate. In the case of solutions of the *n*-butanol – *n*-propylethanoate – *n*-butylethanoate system, there is a predominance of the values of the *n*-propylethanoate activity coefficient. With an increase in the molar mass (molecular sizes) of *n*-alcohol, the values of its activity coefficient in solutions of the systems decrease. The Wilson model more accurately describes the vapour-liquid equilibrium of the solutions of the studied three-component systems. The obtained data are necessary for technological calculations and can be used to further improve the methods for calculating the liquid-vapour equilibrium of multicomponent systems.

Keywords: Liquid-vapour phase equilibria of three-component systems, Wilson and NRTL equations**For citation:** Yu. K. Suntsov, G. Yu. Kharchenko, N. S. Suntsova Liquid-vapour phase equilibria of three-component systems formed by *n*-propanol, *n*-butanol, and *n*-alkylethanoates. *Condensed Matter and Interphases*. 2022;24(2): 273–278. <https://doi.org/10.17308/kcmf.2022.24/9268>**Для цитирования:** Сунцов Ю. К., Харченко Г. Ю., Сунцова Н. С. Фазовые равновесия жидкость-пар трёхкомпонентных систем, образованных *n*-пропанолом, *n*-бутанолом и *n*-алкилетаноатами. *Конденсированные среды и межфазные границы*. 2022;24(2): 273–278. <https://doi.org/10.17308/kcmf.2022.24/9268>✉ Yuri K. Suntsov, e-mail: jsyntsov@mail.ru

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1. Introduction

Data on liquid-vapour phase equilibria are necessary to calculate indicators that determine the direction and speed of technological processes [1]. Solutions of three-component *n*-propanol–*n*-propylethanoate–*n*-butylethanoate and *n*-butanol–*n*-propylethanoate–*n*-butylethanoate systems are often used in the production of *n*-alcohols and ethanoic acid esters [2]. The studies of the phase equilibria of these systems have been fragmentary since they have been carried out solely for technological purposes [3]. As the number of components increases, the volume and complexity of liquid-vapour equilibrium studies increase dramatically. This fact stimulated the development of methods for the calculation of phase equilibria in multicomponent systems based on binary system data. The main achievements in the methods of calculating the phase equilibria have been associated with the development of equations based on local compositions. These equations are based on molecular models of solutions, which provides them with advantages over the polynomial Margules, Redlich–Kister, Van Laar, and Wohl equations. The advantages of the models of local composition are most clearly manifested when predicting the properties of multicomponent systems using the data about their binary components. The Wilson (1) and NRTL (2) equations (Non Random Two Liquid Equation) have been used the most commonly to calculate the vapour-liquid equilibrium of multicomponent systems [1]:

$$\ln \gamma_i = 1 - \ln \left(\sum_{j=1}^n x_j \lambda_{ij} \right) - \sum_{k=1}^n \left[x_k \lambda_{ki} / \sum_{j=1}^n x_j \lambda_{kj} \right], \quad (1)$$

where λ_{ij} and others are parameters of pair interactions.

$$\ln \gamma_i = \sum_{j=1}^n \tau_{ji} G_{ji} x_j / \sum_{k=1}^n x_k G_{ki} + \sum_{j=1}^n \left(x_j G_{ij} / \sum_{k=1}^n x_k G_{kj} \right) \left(\tau_{ij} - \sum_{l=1}^n x_l \tau_{il} G_{il} / \sum_{k=1}^n G_{kl} x_k \right), \quad (2)$$

where: $\tau_{ij} = C_{ij} / RT$; $C_{ij} = g_{ij} - g_{jj}$; $G_{ij} = \exp(-\alpha_{ij} \tau_{ij})$; $G_{ii} = G_{jj} = 1$; $g_{ij} = g_{ji}$; $\alpha_{ji} = \alpha_{ij}$ and for all *i* it is true that $a_{ii} = \tau_{ii} = C_{ii} = 0$; g_{ij} are variables characterising the energy of interaction of the *i*–*j* pairs; g_{jj} is the interaction of *j*–*j* pairs; a_{ij} is a pa-

rameter characterising the degree of ordering of the distribution of molecules in the solution. For solutions of a multicomponent system, it is only necessary to calculate the parameters of pair interactions determined by the experimental data for binary systems.

2. Experimental

During the study of liquid-vapour phase equilibria, water impurities significantly affected the results of the experiment by several hundredths of a percent. Alcohols and esters of chemically pure organic acids were dehydrated using methods [4] and distilled air-free in a laboratory rectifying column. Water in purified reagents was monitored by potentiometric titration using the Fisher reagent [5]. The water content in the reagents did not exceed 0.1%. The criteria for the purity of the purified substances were the boiling point, density, and refractive index. The boiling point of the purified substances was measured in Swietoslowski ebulliometers [1] with an accuracy of ± 0.05 K. The density of the substances was determined by Ostwald pycnometers with an accuracy of ± 0.1 kg/m³, and the refractive index n_D was measured by an IRF-25 refractometer with an accuracy of ± 0.0001 . The constants of purified substances corresponded with the data in [6]. They are given in Table 1. The pressure of saturated vapour and the boiling point of solutions are the most sensitive criteria for the accuracy of calculations of the vapour-liquid equilibrium of systems [1]. The boiling points of the solutions (*T*) at different pressure values (*P*) were measured with a platinum resistance thermometer using the eubuliometric method with an accuracy of ± 0.05 K. The pressure of saturated vapour of the solutions was measured with a mercury manometer using a V-630 cathetometer, with an accuracy of ± 6.66 Pa. Constant pressure in ebulliometers was maintained by an isodromic regulator with negative feedback with an accuracy of ± 6.66 Pa [7]. The obtained experimental data are shown in Tables 3 and 4. Liquid-vapour equilibria of binary systems formed by aliphatic alcohols and esters of organic acids had already been studied [8–24]. The parameter values in the Wilson and NRTL equations for the binary systems were calculated by the method of nonlinear regression [25]. They are presented in Table 2.

Table 1. Properties of purified substances

Substance	Experimental data			Literature data		
	ρ_4^{20}	T, K	n_D^{20}	ρ_4^{20}	T, K	n_D^{20}
<i>n</i> -propanol	0.8044	370.3	1.3854	0.8044	370.30	1.3854
<i>n</i> -butanol	0.8098	391.1	1.3993	0.8098	390.69	1.3993
<i>n</i> -propylethanoate	0.8870	374.7	1.3842	0.8870	374.75	1.3844
<i>n</i> -butylethanoate	0.8825	399.6	1.3940	0.8825	399.65	1.3941

Note: ρ is the density at 293.15 K; T is the boiling point at standard pressure, n_D is the refractive index at 298.15 K

Table 2. Coefficients of binary interaction in the Wilson and NRTL equations, calculated using data about liquid–vapour equilibria, $T = 333 K$

No	System name	Wilson		NRTL		
		λ_{12}	λ_{21}	τ_{12}	τ_{21}	τ_{12}
1	<i>n</i> -propanol - <i>n</i> -propylethanoate	0.8129	0.7116	0.2811	0.3162	0.3236
2	<i>n</i> -propanol- <i>n</i> -butylethanoate	0.554	0.6619	0.6309	0.2099	0.1843
3	<i>n</i> -butanol- <i>n</i> -propylethanoate	0.3838	1.0749	0.0313	0.5025	1.0399
4	<i>n</i> -butanol- <i>n</i> -butylethanoate	0.8417	0.7853	1.2273	0.0995	0.6437
5	<i>n</i> -propanol- <i>n</i> -butanol	1.1432	0.5018	0.2366	-0.5554	0.3835
6	<i>n</i> -propylethanoate- <i>n</i> -butylethanoate	2.3212	0.1319	-1.6022	1.5306	0.9113

The coefficients are oriented towards the first component of the binary system.

Table 3. Activity coefficients and the pressure of saturated vapour of the *n*-propanol (I)–*n*-propylethanoate (II)–*n*-butylethanoate (III) solutions calculated using the Wilson (1) and NRTL (2) model; $T = 333 K$

№	x , mole fractions			γ			P , mm Hg, Experiment	P , mm Hg, Calculated	Equation
	I	II	III	I	II	III			
1	0.9045	0.0473	0.0482	1.0073	1.4810	2.0110	165.2	157.2	(1)
				0.9973	0.8845	1.1877		148.2	(2)
2	0.8041	0.1025	0.0934	1.0284	1.3292	1.7512	156.7	160.3	(1)
				1.0159	0.7511	1.1955		145.1	(2)
3	0.7034	0.1266	0.1700	1.0650	1.2035	1.5625	153.4	158.4	(1)
				1.0586	0.5662	1.2068		139.7	(2)
4	0.6054	0.0795	0.3151	1.1268	1.0828	1.4053	150.8	149.2	(1)
				1.1315	0.2153	1.1618		132.5	(2)
5	0.5104	0.2506	0.2390	1.1638	1.0919	1.3110	156.4	158.9	(1)
				1.1125	0.6323	1.2880		134.8	(2)
6	0.4072	0.3122	0.2806	1.2370	1.0588	1.2170	159.8	156.8	(1)
				1.1467	0.6452	1.3349		131.4	(2)
7	0.3075	0.1100	0.5825	1.4529	0.9723	1.1121	133.3	131.2	(1)
				1.3723	0.1044	1.2964		118.6	(2)
8	0.1830	0.4115	0.4055	1.4801	1.0366	1.0665	146.2	144.2	(1)
				1.2569	0.6164	1.4738		119.9	(2)
9	0.1027	0.1857	0.7116	1.8600	1.0099	1.0198	114.1	111.5	(1)
				1.4795	0.1560	1.5346		108.9	(2)
10	0.1092	0.7231	0.1677	1.3969	1.0409	1.1113	163.7	164.9	(1)
				1.2156	0.8927	1.4363		147.4	(2)

x is the composition of the solution, γ is the activity coefficient; P is the pressure of the saturated vapour of the liquid. See the remaining designations in Table 2.

Table 4. Activity coefficients and the pressure of saturated vapour of solutions of the *n*-butanol (I) – *n*-propylethanoate (II) – *n*-butylethanoate (III) system calculated using the Wilson (1) and NRTL (2) model; $T = 333$ K

No	x , mole fractions			γ			P , mm Hg, Experiment	P , mm Hg, Calculated	Equation
	I	II	III	I	II	III			
1	0.9079	0.0454	0.0467	1.0037	1.5977	1.3779	73.8	70.5	(1)
				1.0126	0.7270	1.0698		63.2	(2)
2	0.8076	0.1080	0.0844	1.0162	1.4875	1.2750	84.9	83.3	(1)
				1.0258	0.7533	1.1259		69.3	(2)
3	0.6929	0.1321	0.1750	1.0414	1.3743	1.1907	90.7	88.0	(1)
				1.0772	0.5440	1.1795		70.5	(2)
4	0.5934	0.0759	0.3307	1.0711	1.2826	1.1405	82.5	80.3	(1)
				1.1981	0.1358	1.1433		69.9	(2)
5	0.5021	0.2547	0.2432	1.1133	1.2443	1.0791	104.3	105.4	(1)
				1.0590	0.7037	1.2835		83.6	(2)
6	0.4003	0.3138	0.2859	1.1704	1.1907	1.0389	113.8	112.1	(1)
				1.0499	0.7227	1.3340		90.1	(2)
7	0.3081	0.1047	0.5872	1.2166	1.1302	1.0318	84.6	84.4	(1)
				1.3229	0.0876	1.3330		79.9	(2)
8	0.2112	0.4115	0.3773	1.3235	1.1185	0.994	124.2	121.3	(1)
				1.0350	0.6998	1.4478		100.1	(2)
9	0.1106	0.1114	0.7780	1.3808	1.0672	1.0016	82.3	83.5	(1)
				1.3244	0.0557	1.4530		88.2	(2)
10	0.1025	0.7571	0.1404	1.5599	1.0557	1.0594	155.4	156.5	(1)
				0.9721	0.9434	1.3978		141.7	(2)

x is the composition of the solution, γ is the activity coefficient; P is the pressure of the saturated vapour of the liquid. See the remaining designations in Table 2.

3. Results and Discussion

The data in Table 2 and equations (1 and 2) were used to calculate the activity coefficients of the components in the solutions of the systems: *n*-propanol–*n*-propylethanoate–*n*-butylethanoate and *n*-butanol–*n*-propylethanoate–*n*-butylethanoate (Tables 3 and 4). The solutions of these systems are often used in the production of alcohols and esters of organic acids. The results of the calculations were verified experimentally. They are given in Tables 3 and 4. The analysis of the data in Tables 3 and 4 established that the Wilson equation more accurately describes the vapour-liquid equilibrium of three-component solutions of the systems. The deviation of the calculated values of the pressure of saturated vapour (P_{calc}) from the corresponding experimental values (P_{exper}) for the three-component systems was: using the Wilson equation $\approx 1.8\%$; using the NRTL equation $\approx 12\%$. The values of the activity coefficient for *n*-propanol and *n*-butanol calculated using the Wilson (1) and NRTL (2) models increased with a

decrease in their concentrations in the solutions of the systems. For example,

1) for the solutions of the *n*-propanol (I)–*n*-propylethanoate (II)–*n*-butylethanoate (III) system calculated using the Wilson equation (1), we had: at $x_1 = 0.9045$, $\gamma_1 = 1.0073$, it increased to $\gamma_1 = 1.8600$ at $x_1 = 0.1027$;

2) for the solutions of the same system calculated using the NRTL equation (2), we had: at $x_1 = 0.9045$, $\gamma_1 = 0.9973$, it increased to $\gamma_1 = 1.4795$ at $x_1 = 0.1027$;

3) for the solutions of the *n*-butanol (I)–*n*-propylethanoate (II)–*n*-butylethanoate (III) system calculated using the Wilson equation (1), we had: at $x_1 = 0.9079$, $\gamma_1 = 1.0037$, it increased to $\gamma_1 = 1.3808$ at $x_1 = 0.1106$;

2) for the solutions of the same system calculated using the NRTL equation (2), we had: at $x_1 = 0.9079$, $\gamma_1 = 1.0126$, it increased to $\gamma_1 = 1.3244$ at $x_1 = 0.1106$.

Similar changes in the values of the activity coefficients of the components in the solutions of the systems were observed for *n*-propylethanoate

and *n*-butylethanoate. When the concentration of ester in the solutions of the systems decreased, the values of their activity coefficients increased (Tables 3 and 4). It should be noted that for *n*-propanol (I) – *n*-propylethanoate (II) – *n*-butylethanoate (III) solutions containing *n*-propylethanoate (II) and *n*-butylethanoate (III) in close concentrations the values of the activity coefficient of *n*-butylethanoate prevailed (Table 3). In the case of solutions of the *n*-butanol – *n*-propylethanoate – *n*-butylethanoate system, there was a predominance of the values of the *n*-propylethanoate activity coefficient (Table 4). With an increase in the molar mass (molecular sizes) of *n*-alcohol, the values of its activity coefficient in solutions of the systems decreased:

1) for the *n*-propanol (I) – *n*-propylethanoate (II) – *n*-butylethanoate (III) system at $x_1 = 0.5104$, $\gamma_1 = 1.1638$;

2) for the *n*-butanol (I) – *n*-butylethanoate (II) – *n*-pentylethanoate (III) system at $x_1 = 0.5021$, $\gamma_1 = 1.1133$.

Spectral and radiographic studies established the presence of hydrogen bonds in *n*-alcohol molecules with an energy of ≈ 30 kJ/mol [26]. The introduction of ester molecules into *n*-propanol and *n*-butanol led to the destruction of the hydrogen bonded structure of the alcohol. For obvious reasons, the disordering effect increased with the increase in the size of ester molecules, which was associated with a decrease in the contribution of *n*-alcohol molecules to the structuring of the solutions of the systems.

4. Conclusions

The Wilson model more accurately describes the vapour-liquid equilibrium of the three-component solutions of the systems. The values of the activity coefficient for *n*-propanol and *n*-butanol calculated using the Wilson and NRTL models increase with a decrease in their concentrations in the system solutions. Similar changes in the values of the activity coefficients of the components in the solutions of the systems were observed for *n*-propylethanoate and *n*-butylethanoate. With an increase in the molar mass (molecular sizes) of *n*-alcohol, the values of its activity coefficient in the solutions of the systems decrease. The obtained data are necessary for technological calculations of rectification processes and can be used to further

improve the methods for calculating the liquid-vapour equilibrium of multicomponent systems.

Author contributions

All authors made an equivalent contribution to the preparation of the publication.

Conflict of interests

The authors declare that they have no known competing financial interests or personal relationships that could have influenced the work reported in this paper.

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