

PHYSICOCHEMICAL STUDIES
OF SYSTEMS AND PROCESSES

**Application of the PC-SAFT Equation of State
to Modeling of Solid–Liquid Equilibria in Systems
with Organic Components Forming Chemical Compounds**

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Abstract—Equilibrium diagrams of liquid and solid phases were calculated by the equation of state, based on the perturbed-chain statistical associating fluid theory (PC-SAFT) for binary and ternary systems constituted by associating substances (water, alcohols, amines, phenol, bisphenol A, acetamide). Phase diagrams were considered for systems in which congruently and incongruently melting intermolecular compounds are formed and for a system with limited mutual solubility of the components in the liquid state. The results of prognostication of phase equilibria were illustrated by the example of a ternary system constituted by bisphenol A, phenol, and water, in which an adduct of bisphenol A and phenol is formed.

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Data on the equilibrium between solid and liquid phases are rather important for analysis of crystallization, which is a method for separation and purification of various substances. Types of solid–liquid equilibrium phase diagrams in binary systems are widely diverse and include, in particular, solid–melt diagrams with limited mutual solubility of the components in the solid (liquid) state and formation of chemical compounds melting with or without decomposition. In the case of diagrams of the latter type, intermolecular compounds, frequently named adducts and hydrates (in aqueous systems) or solvates (in nonaqueous systems), can be formed. In the case of compound formation, liquidus curves corresponding to crystallization of compounds appear in the fusibility diagrams, in addition to the lines of crystallization of pure components. The main experimental technique for obtaining the diagrams mentioned above is differential scanning calorimetry.

In this study, the equation of state, suggested by Gross and Sadowski [1] on the basis of the perturbed-chain statistical associating fluid theory (PC-SAFT), was used to model the solid–liquid phase equilibrium in systems involving chemical compounds. This equation of state is a modification of the known molecular-statistical model SAFT (Statistical Associating Fluid Theory), which has been popular in engineer-

ing calculations recently. It is based on the results of the perturbation theory and a numerical experiment for a fluid formed by chains of solid spheres. The molecular model underlying the PC-SAFT takes into account the formation of chains of solid spheres, dispersion interaction described in terms of the Barker–Henderson perturbation theory [2], and association. It is assumed that there are contact areas on the molecule surface, which are capable of specific interactions with contact areas of other molecules. The PC-SAFT model is being intensively developed; in particular, its variants that take into account multipole interactions in description of polar components have been developed [3–5].

The PC-SAFT model has been successfully tested on various systems, including nonpolar, polar, and associating substances, as well as polymers and copolymers, in a wide range of conditions [1, 3–10].¹ The results obtained are rather promising for further development of this model. However, the consideration has been limited to only fluid phases (liquid–vapor, liquid–liquid, liquid–liquid–vapor). It was of interest to apply this equation to modeling of an equi-

¹ For the software package for calculation of phase equilibria in terms of various models, including SAFT and PC-SAFT, see <http://www.tu-harburg.de/vt2/pe2000/HomePage.html>.

Table 1. Parameters of the PC-SAFT equation for pure associating components

Substance	M , g mol ⁻¹	m	σ , Å	ε/k , K	$\varepsilon^{A_i B_i}$, K	$k^{A_i B_i}$
Water	18.015	1.0656	3.0007	366.51	2500.7	0.034868
Methanol	32.042	1.5255	3.2300	188.90	2899.5	0.035176
<i>n</i> -Octanol	130.23	4.3555	3.7145	262.74	2754.8	0.002197
Hexylamine	101.19	2.8724	4.0036	285.87	1229.0	0.020030
Octylamine	129.24	3.7717	3.9403	272.83	1375.6	0.020101
Phenol	94.113	2.6844	3.5660	250.37	2827.6	0.086578
Acetamide	59.07	2.0233	3.4995	333.91	3441.2	0.030047
Bisphenol A	228.29	9.8321	3.0307	238.92	2763.3	0.030044

librium between solid and liquid phases. The goals of the study were as follows: description of solid-liquid equilibria for a number of binary systems including associating components [water, alcohols, amines, phenol, bisphenol A (BPA), acetamide], which form stable and unstable chemical compounds of varied stoichiometry; description of liquid-liquid and solid-liquid equilibria for the water-phenol system; and prognostication of the fusibility diagram for the ternary mixture of BPA, phenol, and water, in which an adduct of BPA and phenol is formed. Systems in which the solid phase is a solid solution are beyond the scope of this study.

A detailed description of the PC-SAFT equation of state can be found in [1, 3, 6–8], and, therefore, only a brief consideration will be made here. According to the PC-SAFT model, the expression for the compressibility factor z can be written as

$$z = 1 + z^{hc} + z^{disp} + z^{assoc}, \quad (1)$$

where $z = PV/RT$; P , pressure; V , molar volume; R , universal gas constant; and T , temperature. The first term in the sum accounts for the contribution of the ideal gas ($z^{id.gas} = 1$), and the remaining three are related to contributions of chain formation, dispersion component, and association, respectively. Formulas for calculation of z^{hc} and z^{disp} were reported in [1], and the expression for z^{assoc} can be found in [11–13].

Description of i th pure associated substance requires five parameters: number m_i of segments forming the molecule-chain; segment diameter σ_i ; segment interaction energy ε_i/k ; effective association volume $k^{A_i B_i}$, and association energy $\varepsilon^{A_i B_i}/k$ (k is the Boltzmann constant). The last two parameters define the specific interaction between the contact areas A_i and B_i of i th component. When applying the model to mixtures, the Lorenz-Berthelot combina-

tion rules are used, with only a single fitting parameter of the binary interaction, k_{ij} , introduced to correct the dispersion component of interactions in the PC-SAFT equation:

$$\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j), \quad (2)$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j} (1 - k_{ij}). \quad (3)$$

To take into account the association between different-type molecules of i th and j th components, simple mixing rules suggested by Wolbach and Sandler [14] are introduced into the model without an additional fitting parameter:

$$\varepsilon^{A_i B_j} = \frac{1}{2}(\varepsilon^{A_i B_i} + \varepsilon^{A_j B_j}), \quad (4)$$

$$k^{A_i B_j} = \sqrt{k^{A_i B_i} k^{A_j B_j}} \left(\frac{\sqrt{\sigma_{ii} \sigma_{jj}}}{\frac{1}{2}(\sigma_{ii} + \sigma_{jj})} \right)^3. \quad (5)$$

Values of the parameters of the PC-SAFT equation of state for a number of pure associating components (water, alcohols) have been reported in the literature [6], and the lacking parameters for amines, phenol, BPA, and acetamide were determined in this study (Table 1). It was assumed that all molecules of associating components have two specific contact areas each.

Let us now pass to a thermodynamic description of the solid-liquid equilibrium for the case when the solid phase is a pure component, rather than a solid solution. The solubility of a solid in a solvent can be represented, in the case of low pressures and disregarded changes in specific heat, as the expression [15]:

$$x_i^L = \frac{\varphi_{0i}^L}{\varphi_i^L} \exp \left[-\frac{\Delta H_{0i}^m}{RT} \left(1 - \frac{T}{T_{0i}^m} \right) \right], \quad (6)$$

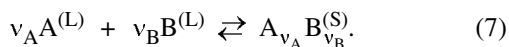
Table 2. Melting point and enthalpy of melting of pure substances

Substance	T_{0i}^m , K	ΔH_{0i}^m , J mol ⁻¹
Water	273.15	6020
Methanol	175.25	3180
<i>n</i> -Octanol	258.03	23700
Hexylamine	252.15	25040
Octylamine	273.37	34740
Phenol	314.0	11510
Acetamide	353.5	15610
Bisphenol A	431.1	30100

where x_i^L is the mole fraction of *i*th component in the liquid phase (superscript L); ΔH_{0i}^m and T_{0i}^m , enthalpy of melting and melting point of pure *i*th component; and φ_{0i}^L and φ_i^L , fugacity coefficients of *i*th pure component and the same component in a mixture at prescribed temperature and pressure.

The values of the fugacity coefficients are calculated using the PC-SAFT equation of state [1]. Solving Eq. (6) for x_i^L at various temperatures, we finally obtain the crystallization line of the pure substance. The thermodynamic properties of the pure substances (H_{0i}^m and T_{0i}^m) considered in this study are listed in Table 2.

If a chemical compound $A_{v_A}B_{v_B}^{(S)}$ (S, superscript denoting the solid phase; v_A and v_B , stoichiometric coefficients) is formed in the system, then the crystallization curve of this compound can be calculated by considering the chemical reaction



Taking the activity of the chemical compound in the solid phase to be unity, we can write for the equilibrium constant K_a

$$K_a = \prod a_i^{v_i} = (x_A \gamma_A)^{-v_A} (x_B \gamma_B)^{-v_B}, \quad (8)$$

with the activity coefficients γ_i in the liquid phase expressed in terms of the ratio between the fugacity coefficients in solution and in *i*th pure liquid as

$$\gamma_i = \varphi_i / \varphi_{0i}. \quad (9)$$

We denote the enthalpy of melting and melting point of the compound by ΔH^{ref} and T^{ref} , respectively. If the compound fully dissociates in the liquid phase, the enthalpy of melting of the compound and the enthalpy of reaction (7) coincide. The temperature de-

pendence of the constant of chemical equilibrium (8) is written as

$$\ln K_a = \ln K_a^{\text{ref}} + \frac{\Delta H^{\text{ref}}}{R} \left(\frac{1}{T^{\text{ref}}} - \frac{1}{T} \right). \quad (10)$$

Expression (10) is the integral form of the equation of the isobar of the chemical reaction. In a narrow temperature range, the enthalpy of reaction (7) can be considered constant and equal to ΔH^{ref} . The temperature T^{ref} may correspond to a congruent or an incongruent point in the fusibility diagram. Occasionally, there are no direct experimental data on values of ΔH^{ref} . Several methods for evaluating this quantity have been suggested in the literature.

(1) Method of weighted-average values of the entropies of melting of the starting compounds [16]; ΔH^{ref} is calculated by the formula

$$\Delta H^{\text{ref}} = T^{\text{ref}} \sum_i x_i \frac{\Delta H_{0i}^m}{T_{0i}^m}, \quad (11)$$

where x_i is the mole fraction of *i*th component in the compound.

(2) ΔH^{ref} and T^{ref} are found by extrapolation to the composition of the compound of the experimentally found concentration dependence of the heat (and temperature) of crystallization of the mixtures [17].

(3) The value of ΔH^{ref} is found by processing of experimental data (melting point–composition) on the assumption of an ideal mixture of monomers and the compound or with account of its nonideality; this value determines the temperature dependence of the association constant [18].

(4) The value of ΔH^{ref} serves as a fitting parameter in processing of experimental data on the crystallization of the compound; in this case, the activity coefficients are calculated using the equation of state [19].

(5) ΔH^{ref} is evaluated using the Schroder equation for ideal solutions [20].

The crystallization line of the chemical compound is calculated using Eqs. (8) and (10), which are solved by the iteration method for the mole fraction of the component in the range from the melting point of the compound (or incongruent point) to the eutectic point. The calculation procedure begins with finding K_a^{ref} at prescribed values of ΔH^{ref} and T^{ref} and molar composition of the chemical compound formed by reaction (7) [19]:

$$K_a^{\text{ref}} = \prod a_i^{v_i} = [x_A \gamma_A(T^{\text{ref}}, x_A)]^{-v_A} [x_B \gamma_B(T^{\text{ref}}, x_B)]^{-v_B}. \quad (12)$$

Table 3. Melting points and enthalpies of melting of intermolecular compounds in the system under consideration

Compound and its stoichiometry	T^{ref} , K	ΔH^{ref} , J mol ⁻¹
Water : methanol = 1 : 1	171.5	8700
Phenol : acetamide:		
1 : 1	307.15	11670
2 : 1	315.45	11770
Hexylamine : <i>n</i> -octanol = 1 : 1	255.03	24480
Octylamine : <i>n</i> -octanol = 1 : 1	267.19	25060
Phenol : bisphenol A:		
1 : 1	375.15	36870
1 : 1, in ternary system (30 mol % water)	359.0	36870
1 : 1, in ternary system (50 mol % water)	343.0	36870

In a particular case in which an adduct of A and B of a stoichiometric composition is formed, $v_A = v_B = 1$ and $x_A = x_B = 0.5$. The activity coefficients $\gamma_A(T^{\text{ref}}, x_A)$ and $\gamma_B(T^{\text{ref}}, x_B)$ are calculated in terms of the PC-SAFT model. After finding K^{ref} from (12), Eqs. (8) and (10) are solved in the next stage of the calculation, at each running value of temperature, lower than T^{ref} , for the unknown quantity x_i^L . Repeating this procedure at other values of T , we can obtain the branch of the crystallization curve of the chemical compound, which intersects the lines corresponding to crystallization of pure components in the system. Table 3 lists the numerical values of T^{ref} and ΔH^{ref} for the chemical compounds formed in the systems under consideration. The optimal values of the binary-interaction parameter k_{ij} , used to describe the phase diagrams, are listed in Table 4.

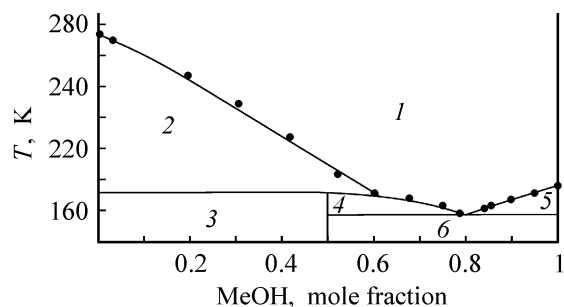


Fig. 1. Fusibility diagram for the system constituted by water and methanol (MeOH) with indication of two-phase region. (T) Temperature; the same for Figs. 3–6. (1 : 1) methanol monohydrate $\text{MeOH} \cdot \text{H}_2\text{O}$. (1) Liquid phase, (2) region of equilibrium between ice and the liquid phase, (3) region of coexistence of ice and crystals of methanol monohydrate, (4) region of equilibrium between $\text{MeOH} \cdot \text{H}_2\text{O}$ crystals and solution, (5) region of coexistence of solid methanol and solution, (6) region of coexistence of two crystalline phases: $\text{MeOH} \cdot \text{H}_2\text{O}$ and methanol. Points, experimental data [18, 21]; lines, calculation by the PC-SAFT equation.

Table 4. Binary interaction parameters evaluated for the systems under study

System	k_{ij}
Water–methanol	–0.18
Phenol–acetamide	–0.055
Hexylamine– <i>n</i> -octanol	–0.06
Octylamine– <i>n</i> -octanol	0.0
Phenol–bisphenol A	–0.01
Phenol–water	–0.018
Bisphenol A–water	–0.018

Let us now discuss the results obtained. The results of modeling of the equilibrium between the solid phase and the liquid for the systems studied are illustrated by Figs. 1–6. Figure 1 shows the fusibility diagram for the methanol–water system in which alcohol monohydrate is formed (1 : 1 stoichiometry). This system shows noticeable negative deviations from the ideal behavior. We carefully checked the sensitivity of the calculation results to the chosen value of ΔH^{ref} , determined by various methods [16, 18, 19]. A testing of the PC-SAFT model demonstrated that the best agreement with the experimental data [18, 21] is provided by ΔH^{ref} equal to 8700 J mol^{-1} , found in [18] using the dimerization model for a nonideal water–methanol solution. The enthalpy of melting of the monohydrate, found using the method of average-weighted values of the entropies of melting of metha-

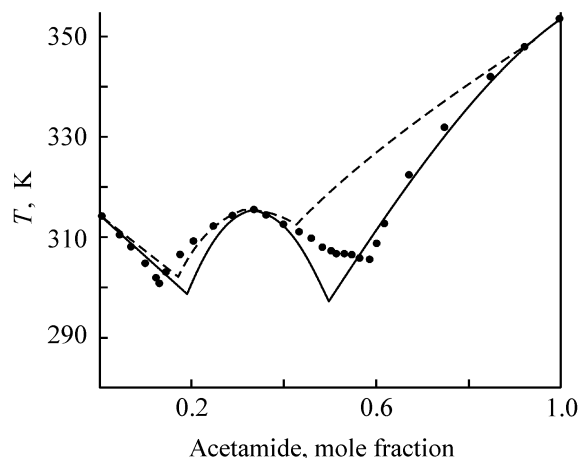


Fig. 2. Melting point vs. composition for the phenol–acetamide system in which two compounds are formed. Points, experimental data [16]; lines, calculation by the PC-SAFT equation at $k_{ij} = -0.055$ (solid lines) and $k_{ij} = 0$ (dashed lines).

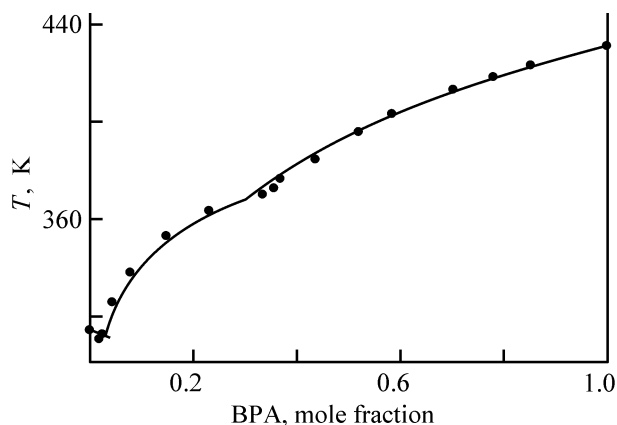


Fig. 3. Liquid–solid equilibrium for the phenol–BPA system. *Points*, experimental data [17]; *lines*, calculation by the PC-SAFT equation.

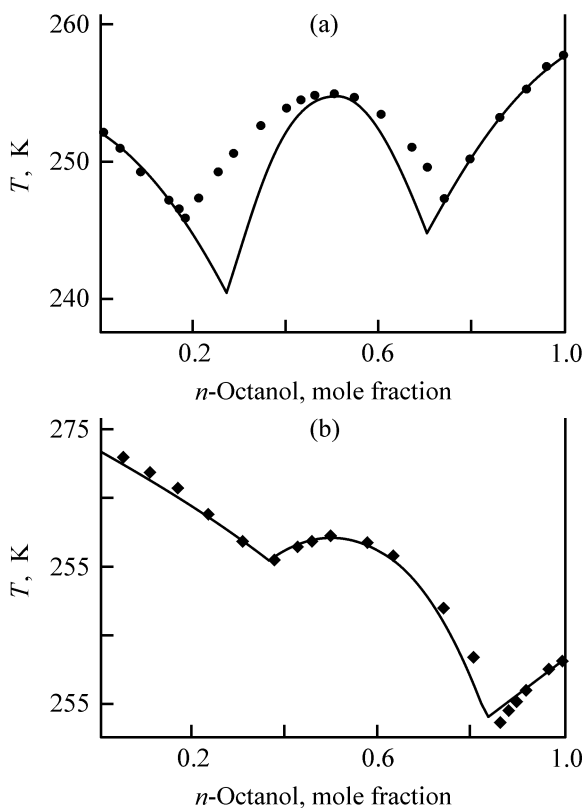


Fig. 4. Fusibility diagrams for the systems (a) hexylamine–*n*-octanol and (b) octylamine–*n*-octanol. *Points*, experimental data [22, 23]; *lines*, calculation by the PC-SAFT equation.

nol and water, is 3440 J mol^{-1} . At this value of ΔH^{ref} and in the case of a varied parameter k_{ij} , a satisfactory description of this system cannot be obtained. It is noteworthy that, at zero k_{ij} , the PC-SAFT equation of state predicts for the methanol–water mixture an in-

correct type of the phase diagram (two crystallization branches of the pure components intersecting at the eutectic point). Figure 2 presents the results of correlation and prognostication in terms of the PC-SAFT model for the phenol–acetamide system, whose phase diagrams show crystallization curves of intermolecular compounds of stoichiometry 2 : 1 and 1 : 1; the crystallization curve of the 1 : 1 compound is very short. To evaluate ΔH^{ref} for both the compounds, we employed the method of weighted-average values of the entropy of melting of the starting substances [16]. The parameter k_{ij} was varied, but, unfortunately, the crystallization line of the 1 : 1 compound could not be described.

The phase diagram of the BPA–phenol system, in which an adduct of equimolar composition is formed, is shown in Fig. 3. The value of ΔH^{ref} of the incongruently melting compound was taken from [17]. This system shows nearly ideal behavior and the model rather well describes it for both zero and slightly negative values of the parameter k_{ij} . The solid–liquid equilibrium was calculated using the PC-SAFT equation of state for the amine–*n*-alcohol systems (Fig. 4), which are characterized by appearance of congruently melting compounds of 1 : 1 stoichiometry [22–24]; the enthalpies of melting of the adducts were determined in [20]. As demonstrated by Fig. 4a, the calculation correctly reproduces the general form of the diagram, but the calculated crystallization lines of the adduct somewhat differ from those obtained experimentally. This system exhibits strong negative deviations from the Raoult law. The results of prognostication by the PC-SAFT equation for the octylamine–octanol system (Fig. 4b), whose behavior is nearly ideal, coincide with the experimental data with good precision.

Recently, experimental data have been reported [25] on the solid–liquid equilibrium for the BPA–phenol–water ternary system in which an adduct of BPA and phenol is formed with a 1 : 1 stoichiometry. To prognosticate the phase diagram for this system, additional calculations of fusibility diagrams were performed for phenol–water and BPA–water binary subsystems.

As is known [26], the phase behavior of the phenol–water system is rather complex: the liquid solution stratifies and three-phase equilibria of different types appear. Figure 5 illustrates the phase diagram for this system under atmospheric pressure, with the solid–liquid, liquid–liquid, and liquid–vapor equilibria shown. It is noteworthy that the regions of coexistence of ice and the liquid phase (L_2) and of solid phenol

and liquid (L_2) are rather narrow and virtually invisible on the scale used in the figure. The PC-SAFT equation can reflect with an acceptable accuracy the full phase diagram of this system in a wide temperature range. Unfortunately, no experimental data on the solid-liquid equilibrium could be found in the literature, and, therefore, the fusibility diagram of this mixture was prognosticated ($k_{ij} = 0$). The predicted diagram was found to be similar to that for the phenol-water system.

Figure 6 shows the results of description of the phase diagram of the ternary system BPA-phenol-water for a constant mole fraction of water. The dependence of the melting point on composition was plotted for this system on the scale of a relative mole fraction of BPA (characterizing the composition of the BPA-water quasibinary mixture) at a prescribed content of water. The calculations for the ternary system used the same value of ΔH^{ref} as that for the BPA-phenol binary subsystem. T^{ref} were found by extrapolation from experimental data on the dependence of the melting point of the ternary mixture on its composition. The crystallization lines of the pure substances and adduct were prognosticated for the ternary aqueous-organic system for a zero value of the parameter k_{ij} for the BPA-water mixture; a calculation was also made with fitting of this parameter by using the data for the BPA-phenol-water system ($k_{ij} = -0.018$). The use of a corrected value of k_{ij} for the BPA-water binary subsystem made it possible to describe the experimental data with a good accuracy. As can be seen in Fig. 6, the crystallization curves in the ternary system shift to lower temperatures as the content of water increases.

CONCLUSIONS

(1) The PC-SAFT model describes, on the whole, successfully the solid-liquid equilibrium for binary and ternary systems (methanol-water, phenol-acetamide, bisphenol A-phenol, hexylamine-octanol, octylamine-octanol, and bisphenol A-phenol-water) in which intermolecular compounds are formed. Use of a single fitting parameter, that of the binary interaction, is sufficient for a satisfactory description of phase diagrams for all of the systems considered.

(2) The model reproduces with an acceptable accuracy the phase diagram of the phenol-water system at atmospheric pressure, in which various types of two- and three-phase equilibria are observed.

(3) The lines of crystallization lines of a chemical compound that completely dissociates in the liquid

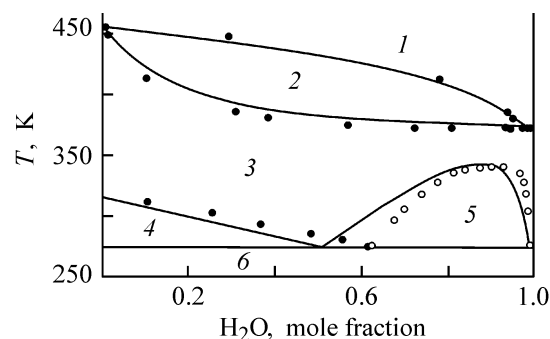


Fig. 5. Phase diagram of the phenol-water system under atmospheric pressure. (1) Vapor phase, (2) region of vapor-liquid equilibrium, (3) liquid phase, (4) region of coexistence of solid phenol and solution, (5) region of a liquid (L_1)-liquid (L_2) equilibrium, (6) region of coexistence of phenol crystals and ice. Points, experimental data [26]; lines, calculation by the PC-SAFT equation.

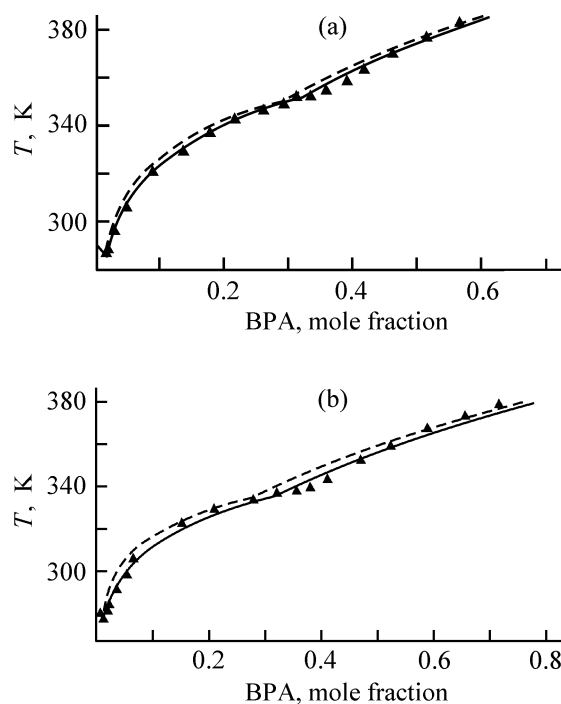


Fig. 6. Prognostication of the fusibility diagrams of the BPA-phenol-water ternary system at water content of (a) 30 mol % and (b) 50 mol %. (BPA) Relative content of bisphenol A in the BPA-phenol quasibinary system. Points, experimental data [25]; lines, calculation by the PC-SAFT equation for the following values of the parameter k_{ij} for the BPA-water binary subsystem: $k_{ij} = -0.018$ (solid lines) and $k_{ij} = 0$ (dashed lines).

phase can be calculated using the method described in this study from data on the enthalpy of melting and the melting point of the compound.

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