

PHYSICOCHEMICAL STUDIES  
OF SYSTEMS AND PROCESSES

Equations and Determination of Physicochemical Properties  
of Ammonium Sulfate-Nitrate Solutions

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Received July 6, 2005; in final form, June 2006

**Abstract**—Theoretical and correlation equations for calculation of multicomponent systems were considered in terms of a previously developed theory of ion-ion interactions in steady- and nonsteady-state processes for the example of ammonium sulfate-nitrate solutions formed from effluent gases of thermal power plants.

**DOI:** 10.1134/S1070427207020097

Effluent gases of thermal power plants contain a significant amount of sulfur dioxide ( $\sim 7 \text{ g m}^{-3}$ ) and nitrogen oxides ( $\sim 1.5 \text{ g m}^{-3}$ ), which are discharged into the atmosphere and contaminate air, soil, and water basins. Previously a new technology for manufacture of ammonium sulfate-nitrate (ASN) fertilizers from these contaminants has been developed [1–3]. The technology includes introduction of gaseous ammonia, electron-beam processing of dusty effluent gases, absorption of the forming  $\text{SO}_3$  and  $\text{NO}_2$  by water, concentration of ASN solutions, evaporation, and granulation.

Development of new technologies and choice of the optimal ways of utilization of industrial waste require that thermodynamics, kinetics, and various physicochemical parameters should be known. The technology suggested requires particularly reliable and authentic data on physicochemical properties of concentrated solutions of inorganic substances.

The theory of interparticle interactions in steady-state processes in concentrated electrolyte solutions [4] and some implications of this theory [5] were used to suggest methods for determination of physicochemical parameters of multicomponent systems. The following properties of the solutions were analyzed: density, specific heat, thermal conductivity, water vapor

pressure over solution, activity of water, surface tension, dynamic viscosity coefficient, electrical conductivity, and boiling and freezing points.

The present study is devoted to analysis of the physicochemical properties of solutions of multicomponent systems based on  $(\text{NH}_4)_2\text{SO}_4$  and  $\text{NH}_4\text{NO}_3$ , with minor additions of  $\text{NH}_4\text{HSO}_3$ ,  $\text{NH}_4\text{HSO}_4$ ,  $(\text{NH}_4)_2\text{SO}_3$ , and  $\text{NH}_4\text{NO}_2$ . The concentrations of the components in solutions was varied from 10 to 70 wt % at an  $(\text{NH}_4)_2\text{SO}_4/\text{NH}_4\text{NO}_3$  ratio equal to 4 and temperatures of 25–80°C.

The density of a multicomponent solution was calculated by the formula

$$\rho = \rho_0 + \sum_{i=1}^h c_i (A_{1i} + A_{2i}t + A_{3i}c_i), \quad (1)$$

where  $\rho$  is the solution density ( $\text{kg m}^{-3}$ );  $\rho_0$ , water density ( $\text{kg m}^{-3}$ );  $h$ , number of solution components;  $c_i$ , electrolyte concentration (wt %);  $t$ , temperature (°C); and  $A_{ij}$ , coefficients found by processing by methods of regression analysis of the authors' own data and those published in the literature for a large number of electrolytes [5]. The values of these coefficients for the components of the ASN solution are listed in Table 1.

**Table 1.** Coefficients of Eq. (1)

Electrolyte	$A_{1i}$	$A_{2i}$	$A_{3i}$	$c$ , wt %	$t$ , °C	$S_p^*$ , $\text{kg m}^{-3}$	$\Delta^*$ , %
$\text{NH}_4\text{NO}_3$	4.1148	-0.0101	0.0165	0–70	0–100	4.15	0.26
$(\text{NH}_4)_2\text{SO}_4$	5.8719	-0.0012	-0.0020	0–70	0–100	1.89	0.13

\*  $S_p$  is the root-mean-square error, and  $\Delta$ , average relative error of calculation.

**Table 2.** Density  $\rho$  of ASN solutions

$c$ , wt %	$\rho$ , kg m <sup>-3</sup> , at indicated temperature, °C						
	25	30	40	50	60	70	80
10	1052.4	1050.9	1047.5	1043.2	1038.3	1032.8	1026.8
20	1107.5	1106.1	1102.6	1098.4	1093.5	1088.0	1082.0
30	1162.6	1161.2	1157.8	1153.6	1148.6	1143.1	1137.1
40	1217.8	1216.4	1212.9	1208.6	1203.7	1198.2	1192.2
50	1272.5	1271.4	1268.0	1263.7	1258.8	1253.3	1247.3
60	1327.9	1326.5	1323.0	1318.8	1313.9	1308.3	1302.3
70	1383.0	1381.6	1378.1	1373.8	1368.9	1363.4	1357.3

**Table 3.** Coefficients of Eq. (3)

Electrolyte	$B_{1i}$	$B_{2i} \times 10^2$	$B_{3i} \times 10^2$	$B_{4i} \times 10^3$	$c$ , wt %	$t$ , °C	$S_{Cp}$ , J kg <sup>-1</sup> K <sup>-1</sup>	$\Delta$ , %
NH <sub>4</sub> NO <sub>3</sub>	-39.21	31.0495	-19.0210	-2.0051	4–16	20–10	13.76	0.25
(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	-55.40	5.3285	96.0142	0.3568	0–15	10–10	10.20	0.1
	-43.30	4.3392	21.5319	0.0312	15–60	10–10	11.46	0.29

The density of water (kg m<sup>-3</sup>) on the saturation line at 0–150°C was calculated with a relative error of  $4.8 \times 10^{-3}\%$  by the formula

$$\rho_0 = 999.810745 + R_1 t^* + R_2 t_*^{1.5} + R_3 t_*^2 + R_4 t_*^{2.5} + R_5 t_*^3 + R_6 t_*^{3.5} + R_7 t_*^4 + R_8 t_*^{4.5}, \quad (2)$$

where  $t^* = 0.01t$ ,  $R_1 = 15.910174$ ,  $R_2 = -73.840671$ ,  $R_3 = 141.693443$ ,  $R_4 = -297.162815$ ,  $R_5 = 160.758796$ ,  $R_6 = 146.727674$ ,  $R_7 = -194.580793$ ,  $R_8 = 58.847919$ .

The results obtained in calculating the density of the ASN solution are listed in Table 2.

The specific heat of the multicomponent solution,  $C_p$  (J kg<sup>-1</sup> K<sup>-1</sup>) can be calculated by the formula

$$C_p = C_{p0} + \sum_{i=1}^k (B_{1i} + B_{2i}c_i + B_{3i}t + B_{4i}t^2)c_i. \quad (3)$$

Here,  $C_{p0}$  is the specific heat of water (J kg<sup>-1</sup> K<sup>-1</sup>);  $\tilde{c}_i$ , concentration of  $i$ th component in a binary isopiestic solution (wt %);  $t$ , temperature (°C);  $c_i$ , concentration of  $i$ th component in the multicomponent solution (wt %);  $k$ , number of the solution components; and  $B_{ni}$ , coefficients found by processing by methods of regression analysis of the authors' own data and those published in the literature for a large number of electrolytes [6, 7]. The values of these coefficients for the components of the ASN solution are listed in Table 3.

The specific heat of water (J kg<sup>-1</sup> K<sup>-1</sup>) on the saturation line at  $0^\circ\text{C} \leq t < 40^\circ\text{C}$  was calculated with a root-mean-square and average relative calculation errors of 3.95 J kg<sup>-1</sup> K<sup>-1</sup> and 0.035%, respectively, by the formula

$$C_{p0} = 4.21703 - 0.068372t_*^{0.5} - 0.193808t_*^{1.5} + 0.340252t_*^2, \quad (4)$$

where  $t_* = 0.01t$ .

In the temperature range  $40^\circ\text{C} \leq t < 250^\circ\text{C}$ , the specific heat of water was found by the formula

$$C_{p0} = 4.178232 - 0.200822t_*^{2.5} + 0.551896t_*^{1.3} - 0.435824t_*^{3.5} + 0.123167t_*^4. \quad (5)$$

The value of  $\tilde{c}_i$  was calculated as

$$\tilde{c}_i = E_i^{-1} \sum_{j=1}^k E_j c_j. \quad (6)$$

Here  $E_i$  is a coefficient characterizing the vapor pressure over solution, which can be found from the dependence [5, 7]:

$$E_i = (1 - a_w^s)c_i^s, \quad (7)$$

where  $a_w^s$  and  $c_i^s$  are, respectively, the activity of water and the mass fraction of a saturated solution of a separate component of the system under consideration at a given temperature.

**Table 4.** Specific heat of ASN solutions,  $C_p$ 

$c$ , wt %	$C_p$ , J kg <sup>-1</sup> K <sup>-1</sup> at indicated temperature, °C						
	25	30	40	50	60	70	80
10	4175.1	4173.3	4173.3	4174.9	4178.0	4182.6	4189.0
20	4170.2	4168.3	4167.8	4168.9	4171.5	4175.5	4181.3
30	4165.4	4163.2	4162.3	4163.0	4164.9	4168.5	4173.6
40	4160.6	4158.2	4156.8	4157.0	4158.4	4161.4	4165.9
50	4155.7	4153.1	4151.3	4151.0	4151.9	4154.3	4158.2
60	4150.9	4148.1	4145.8	4145.0	4145.4	4147.2	4150.5

**Table 5.** Coefficients of Eq. (8)

Electrolyte	$-\beta \times 10^3$	$c$ , wt %	$t$ , °C	$S_\lambda \times 10^3$ , W m <sup>-1</sup> K <sup>-1</sup>	$\Delta$ , %	Electrolyte	$-\beta \times 10^3$	$c$ , wt %	$t$ , °C	$S_\lambda \times 10^3$ , W m <sup>-1</sup> K <sup>-1</sup>	$\Delta$ , %
NH <sub>4</sub> NO <sub>3</sub>	1.1598	0–50	10–100	5.97	0.79	(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	2.3668	0–30	10–90	9.69	1.22

**Table 6.** Thermal conductivity  $\lambda$  of ASN solutions

$c$ , wt %	$\lambda$ , W m <sup>-1</sup> K <sup>-1</sup> at indicated temperature, °C						
	25	30	40	50	60	70	80
10	0.594	0.602	0.617	0.630	0.640	0.649	0.656
20	0.581	0.589	0.604	0.616	0.626	0.635	0.641
30	0.569	0.576	0.590	0.602	0.613	0.621	0.627

The results obtained in calculating the specific heat of the ASN solution are listed in Table 4.

The thermal conductivity of multicomponent electrolyte solutions was calculated by the formula

$$\lambda = \lambda_0 \left( 1 + \sum_{i=1}^k \beta_i c_i \right). \quad (8)$$

Here,  $\lambda$  is the thermal conductivity of the solution (W m<sup>-1</sup> K<sup>-1</sup>);  $\lambda_0$ , thermal conductivity of water (W m<sup>-1</sup> K<sup>-1</sup>);  $c_i$ , concentration of  $i$ th component in the multicomponent solution (wt %);  $k$ , number of solution components; and  $\beta_i$ , coefficients found by processing by methods of regression analysis the authors' own data and those published in the literature for a large number of electrolytes [8]. The values of these coefficients for the components of the ASN solution are listed in Table 5.

The thermal conductivity of water on the saturation line at temperatures of 0 to 135°C was approximated

with a root-mean-square calculation error  $S_\lambda = 0.29$  W m<sup>-1</sup> K<sup>-1</sup> and average relative calculation error  $\Delta = 0.03\%$  with the polynomial

$$\lambda_0 = 10^{-3}(L_0 + L_1 T^* + L_2 T_*^{1.5} + L_3 T_*^{2.5} + L_4 T_*^3), \quad (9)$$

where  $L_0 = 560.971778$ ,  $L_1 = 178.153112$ ,  $L_2 = 59.731618$ ,  $L_3 = -245.008302$ ,  $L_4 = 124.973313$ ,  $T^* = 0.01t$ , and  $t$  is temperature (°C).

The results of calculation of the thermal conductivity of an ASN solution are listed in Table 6.

The water vapor pressure (Pa) over a multicomponent electrolyte solution was calculated by the equation

$$P = P_0 \exp \left( 2.3026 \sum_{i=1}^k m_i P_i^* \right), \quad (10)$$

where  $P_0$  is the water vapor pressure over pure water (Pa);  $m_i$ , mass concentration of the electrolyte in

**Table 7.** Coefficients of Eq. (15)

Coefficient	<i>c</i> , wt %	<i>t</i> , °C	Δ, %	Coefficient	<i>c</i> , wt %	<i>t</i> , °C	Δ, %
NH <sub>4</sub> NO <sub>3</sub> electrolyte				(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub> electrolyte			
$W_{0i} = -9.0900 \times 10^{-3}$	} 2–50	} 0–100	} 0.46	$W_{0i} = -1.6377 \times 10^{-2}$	} 2–50	} 0–100	} 0.17
$W_{1i} = 6.2000 \times 10^{-5}$				$W_{1i} = 9.9500 \times 10^{-5}$			
$W_{2i} = 7.5700 \times 10^{-5}$				$W_{2i} = -2.3900 \times 10^{-5}$			
$W_{3i} = -9.0000 \times 10^{-7}$				$W_{3i} = -8.0000 \times 10^{-7}$			
$W_{4i} = -7.6000 \times 10^{-6}$				$W_{4i} = -2.0900 \times 10^{-5}$			
$W_{5i} = 0.1000 \times 10^{-6}$				$W_{5i} = 2.0000 \times 10^{-7}$			

**Table 8.** Water vapor pressure *P* over an ASN solution

<i>c</i> , wt %	<i>P</i> , Pa, at indicated temperature, °C						
	25	30	40	50	60	70	80
10	3079	4127	7179	12010	19394	30329	46065
20	2970	3982	6931	11597	18727	29279	44445
30	2829	3794	6606	11057	17856	27914	42366
40	2643	3543	6168	10325	16678	26083	39611
50	2385	3194	5554	9294	15022	23530	35823
60	2014	2689	4655	7778	12590	19809	30382

the solution (mol kg<sup>-1</sup>); *k*, number of solution components; and  $P_i^*$ , correction for the decrease in the water vapor pressure over the multicomponent electrolyte solution.

The water vapor pressure over pure water on the saturation line is calculated with root-mean-square and average relative errors of 39.54 Pa and 0.006% by the formula

$$P_0 = P_c \exp B. \quad (11)$$

Here,  $P_c$  is the critical pressure equal to  $2.2064 \times 10^7$  Pa and *B* is given by

$$B = T_c A/T, \quad (12)$$

where  $T_c$  is the critical temperature equal to 647.14; *T*, temperature (K); and *A* is found from the following dependence at temperature of 0 to 100°C:

$$A = A_0 + A_1 T_*^{1.5} + A_2 T_*^3 + A_3 T_*^{3.5}, \quad (13)$$

$A_0 = -0.595684$ ,  $A_1 = -11.039345$ ,  $A_2 = 17.449275$ ,  $A_3 = -16.028445$ ,

$$T_* = 1 - T/T_c. \quad (14)$$

The value of  $P_i^*$  in Eq. (10) was found using the formula

$$P_i^* = W_{0i} + W_{1i} t_i + W_{2i} m_i + W_{3i} t_i^2 + W_{4i} t_i m_i + W_{5i} t_i^2 m_i, \quad (15)$$

where the coefficients  $W_{ji}$  are found by processing by methods of regression analysis of the authors' own data and those published in the literature for a large number of electrolytes [5]. The values of these coefficients for the components of the ASN solution are listed in Table 7.

The results obtained by calculating the water vapor pressure over an ASN solution are listed in Table 8.

The activity of water can be calculated by theoretical and semiempirical equations reported in [4, 5], where various calculation examples were demonstrated. In view of the limited volume of the present communication, the following formula can be recommended in the given case

$$a_w = \exp(2.3026 \sum_{i=1}^k m_i P_i^*). \quad (16)$$

**Table 9.** Activity  $a_w$  of water over an ASN solution

$c$ , wt %	$a_w$ at indicated temperature, °C						
	25	30	40	50	60	70	80
10	0.9725	0.9729	0.9735	0.9737	0.9737	0.9733	0.9727
20	0.9379	0.9387	0.9397	0.9403	0.9402	0.9396	0.9385
30	0.8935	0.8944	0.8957	0.8964	0.8964	0.8958	0.8946
40	0.8345	0.8352	0.8364	0.8371	0.8373	0.8371	0.8364
50	0.7531	0.7530	0.7531	0.7535	0.7542	0.7551	0.7564
60	0.6360	0.6339	0.6312	0.6306	0.6321	0.6357	0.6416

**Table 10.** Surface tension  $\sigma$  of ASN solutions

$c$ , wt %	$\sigma$ , N m <sup>-1</sup> , at indicated temperature, °C						
	25	30	40	50	60	70	80
10	0.073	0.072	0.071	0.069	0.067	0.066	0.064
20	0.075	0.074	0.073	0.071	0.069	0.067	0.066
30	0.077	0.076	0.075	0.073	0.071	0.070	0.068
40	0.080	0.079	0.078	0.076	0.074	0.072	0.071
50	0.084	0.083	0.082	0.080	0.078	0.076	0.075
60	0.090	0.089	0.088	0.086	0.084	0.082	0.080

**Table 11.** Coefficients of Eq. (19)

Electrolyte	$A_0 \times 10^3$	$A_1 \times 10^4$	$A_2 \times 10^5$	$A_3 \times 10^6$	$c$ , wt %	$t$ , °C	$S_\eta \times 10^2$	$\Delta$ , %
NH <sub>4</sub> NO <sub>3</sub>	-13.765	3.956	13.88	-2.1	5-40	25-95	1.50	1.32
(NH <sub>4</sub> ) <sub>2</sub> SO <sub>4</sub>	15.434	0.744	12.29	0.0	0-50	20-90	3.54	1.72

The results obtained by calculating the activity of water over the ASN solution are listed in Table 9.

The surface tension of a multicomponent solution can be calculated by the formula [8]:

$$\sigma = \sigma_0 + 0.049(1 - a_w), \quad (17)$$

where  $\sigma$  is the surface tension of the multicomponent electrolyte solution (N m<sup>-1</sup>);  $\sigma_0$ , surface tension of water (N m<sup>-1</sup>); and  $a_w$ , activity of water in the multicomponent solution.

The surface tension was calculated with high accuracy for the entire range of existence of water from the data of [9]:

$$\sigma_0 = B \left( \frac{T_0 - T}{T_0} \right)^m \left[ 1 + b \left( \frac{T_0 - T}{T_0} \right) \right], \quad (18)$$

where  $B = 235.6 \times 10^{-3}$ ,  $T_0 = 647.15$ ,  $m = 1.256$   $b = -0.625$ .

The results of calculation of the surface tension of ASN solutions are listed in Table 10.

The dynamic viscosity coefficient  $\eta$  (Pa s) of a multicomponent solution was calculated by the formula

$$\eta = \eta_0 \exp V, \quad (19)$$

$$V = \sum_{i=1}^k c_i (A_{0i} + A_{1i}t + A_{2i}c_i + A_{3i}t^2),$$

where  $\eta_0$  is the dynamic viscosity coefficient of water (Pa s);  $k$ , number of electrolyte components in the solution;  $c_i$ , mass fraction of  $i$ th component in the multicomponent solution (%);  $t$ , temperature (°C); and  $A_{ij}$ , found by processing by methods of regression analysis of the authors' own data and those published in the literature for a large number of electrolytes [10, 11]. The values of these coefficients for the components of the ASN solution are listed in Table 11.

The viscosity of water,  $\eta_0$  (Pa s), on the saturation line in the temperature range 0–350°C was calcu-

**Table 12.** Dynamic viscosity coefficient  $\eta$  of ASN solutions

$c$ , wt %	$\eta \times 10^{-3}$ , Pa s, at indicated temperature, °C						
	25	30	40	50	60	70	80
10	1.018	0.919	0.762	0.645	0.555	0.483	0.426
20	1.187	1.077	0.904	0.773	0.670	0.589	0.523
30	1.407	1.284	1.089	0.941	0.824	0.730	0.654
40	1.696	1.557	1.335	1.165	1.030	0.920	0.830
50	2.080	1.920	1.665	1.467	1.309	1.179	1.072
60	2.593	2.408	2.110	1.879	1.691	1.537	1.408

lated with root-mean-square and average relative calculation errors of, respectively, 1.19 (Pa s) and 0.07% in the temperature interval 0–200°C by the formula

$$\eta_0 = S_0 + S_1 t + S_2/t + S_3 \exp(-0.1t) + S_4/t^2 + S_5 \sqrt{t} + S_6 \ln t, \quad (20)$$

where  $S_0 = 4496.839782$ ,  $S_1 = -4.644252$ ,  $S_2 = -7025.494506$ ,  $S_3 = -159.419139$ ,  $S_4 = 4104.442382$ ,  $S_5 = 316.705387$ , and  $S_6 = -1486.934219$ .

The results of a calculation of the dynamic viscosity coefficient of ASN solutions are listed in Table 12.

The electrical conductivity  $\Lambda$  ( $\text{S cm}^2 \text{ mol}^{-1}$ ) of a multicomponent electrolyte solution can be calculated using the following theoretical equation [4–6]:

$$\Lambda = \frac{1}{c_{kg}} \sum_{i=1}^k v_i c_{ki} [\Lambda_i (1 - L_i) + K_{1i} c_{ki}^2]. \quad (21)$$

Here,  $c_{kg}$  is the total molar concentration of the equivalent of the solution components ( $\text{g-equiv dm}^{-3}$ );  $k$ , number of electrolyte components in the solution;  $v_i$ , number of like charges of the electrolyte molecule;  $c_{ki}$ , molar concentration of each electrolyte component ( $\text{mol dm}^{-3}$ );  $\Lambda_i^0$ , limiting molar electrical conductivity of each component of the multicomponent solution in water ( $\text{S cm}^2 \text{ mol}^{-1}$ );  $L_i$ , parameter of  $i$ th component in the solution; and  $K_{1i}$ , correction factor for  $i$ th component of the solution [4, 5].

In turn,  $\Lambda_i^0$  was found using the formula

$$\Lambda_i^0 = \lambda_i^0 + \lambda_j^0, \quad (22)$$

where  $\lambda_i^0$  and  $\lambda_j^0$  are the limiting electrical conductivities of cations and anions in water ( $\text{S cm}^2 \text{ mol}^{-1}$ ).

The limiting molar electrical conductivities of cations and anions in water were calculated using expressions reported in [5].

The parameter  $L_i$  was found using the equation

$$L_i = V_{0i} + V_{1i} t + V_{2i} c_{ki} + V_{3i} t c_{ki} + V_{4i} (t c_{ki})^2 + V_{5i} c_{ki}^{0.7} + V_{6i} c_{ki}^{0.7} + V_{7i} (t c_{ki})^{0.5}, \quad (23)$$

where  $t$  is temperature (°C), and  $V_{ij}$  are coefficients found by processing by methods of regression analysis of the authors' own data and those published in the literature for a large number of electrolytes [5].

The correction factor  $K_{1i}$  was determined by the formula [5]:

$$K_{1i} = -3.161 \times 10^{17} \frac{(v_k z_i)^2 \alpha_a}{\eta_0 \varepsilon (\varepsilon T)^3 (6 - \alpha_a^2)}, \quad (24)$$

where  $v_k$  is the number of ions in the electrolyte molecule;  $z_i$ , cation charge;  $\alpha_a$ , theoretical parameter [4, 6];  $\eta_0$ , viscosity of water (Pa s);  $\varepsilon$ , dielectric constant; and  $T$ , temperature (K).

The value of  $\alpha_a$  was found using the expression derived in [4]:

$$\alpha_a = \sinh(\beta/a), \quad (25)$$

where  $\beta$  is calculated by the formula

$$\beta = \frac{1.6718 \times 10^{-3} |z_i z_j|}{\varepsilon T}. \quad (26)$$

The value of  $\varepsilon$  can be calculated with a standard deviation of 0.33 in  $\varepsilon$  units by the equation [12]:

$$\varepsilon = 1 + (a_1/T^*)\rho + (a_2/T^* + a_3 + a_4 T^*)\rho^2 + (a_5/T^* + a_6 T^* + a_7 T^2)\rho^3 + (a_8/T^2 + a_9/T^* + a_{10})\rho^4, \quad (27)$$

where

$$T^* = T/298.15, \quad \rho^* = \rho_0/1000, \quad (28)$$

and  $\rho_0$  is the density of water ( $\text{kg m}^{-3}$ ).

**Table 13.** Electrical conductivity  $\Lambda$  of ASN solutions

$c$ , wt %	$\Lambda$ , S cm <sup>2</sup> mol <sup>-1</sup> , at indicated temperature, °C						
	25	30	40	50	60	70	80
10	32.81	35.92	42.14	48.47	54.98	61.74	68.78
20	31.13	33.96	39.59	45.27	51.10	57.12	63.38
30	29.36	31.93	37.04	42.17	47.43	52.87	58.52
40	27.69	30.04	34.70	39.39	44.20	49.18	54.37
50	26.15	28.31	32.59	36.91	41.36	45.99	50.82
60	24.74	26.74	30.70	34.72	38.88	43.21	47.75

The coefficients  $a_i$  have the following values:  $a_1 = 7.62571$ ,  $a_2 = 244.003$ ,  $a_3 = -140.569$ ,  $a_4 = 27.7841$ ,  $a_5 = -96.2805$ ,  $a_6 = 41.7909$ ,  $a_7 = -10.2099$ ,  $a_8 = -45.2059$ ,  $a_9 = 84.6395$ ,  $a_{10} = -35.8644$ .

Equation (27) is applicable under the following conditions: temperature 273.15–823.15 K, density 0–1150 kg m<sup>-3</sup>, pressure 0–500 MPa. The value of  $a$  in Eq. (25) is found by the formula

$$a = \chi_f(a_i + a_j), \quad (29)$$

where  $\chi_f = 1$  for electrolytes of the symmetric type and  $\chi_f = 2$  for those of the asymmetric type, and distances from the ion center to the oxygen of water for ions in solution and the effective radii of polyatomic ions  $a_i$  and  $a_j$  (nm) can be found in [5].

The results of calculation of the electrical conductivity of ASN solutions are listed in Table 13.

The boiling point  $T_b$  (K) of a multicomponent solution can be calculated with an accuracy acceptable for practical purposes by the modified formula [5]:

$$T_b = 500.2238 / [(24.6536 + \ln a_w)^{1/2} - 3.6249], \quad (30)$$

$$0 < t < 215^\circ\text{C}, S_{T_b} = 0.6 \text{ K},$$

where  $S_{T_b}$  is the root-mean-square calculation error (K).

Equation (30) is solved by the method of iterations. First  $a_w$  (0.99) is set and  $T_b$  is calculated. This value of  $T_b$  is used to find  $a_w$ , using formulas (10)–(16) or some others. Then,  $T_b$  is again calculated [calculation of the vapor pressure over solution with the use of coefficients in formulas (13) and (15) allows a slight extrapolation beyond 100°C]. The number of iterations is 2. Making this number larger impairs the calculation accuracy. Instead of calculating  $a_w$ , it is possible to use its experimental values reported in [13] at temperatures below 100°C for many tens of electrolytes, with the activity of water at  $T_b$  found by

means of a linear approximation. The results of calculation of the boiling points of ASN solutions are presented below (°C):

$c$ , wt %	10	20	30	40	50	60
$T_b$ , °C	100.86	101.97	103.28	105.16	107.97	112.42

The freezing temperature of a multicomponent solution,  $T_f$  (K) is commonly found in the entire range of activities of water, using the equation [5]:

$$T_f = \frac{555.316}{2.76375 - \sqrt{\ln a_w^{(25)} + 0.53398}}, \quad (31)$$

where  $\ln a_w^{(25)}$  is the activity of water over solution at 25°C.

The applicability of formula (31) is limited by the lower bound of the interval  $|\ln a_w^{(25)}| < 0.53398$ , because the expression within the square root should be positive.

The results of calculation of the freezing point of ASN solutions are presented below (°C):

$c$ , wt %	10	20	30	40	50
$T_f$ , °C	-2.58	-5.95	-10.54	-17.19	-27.79

The whole set of the physicochemical studies performed enabled optimal consideration of heat-and-mass exchange processes in the technology for manufacture of a complex integrated fertilizer based on ammonium sulfate and nitrate with microelements from effluent gases discharged by thermal power plants.

## CONCLUSIONS

(1) The previously developed theory of ion–ion interactions in steady- and nonsteady-state processes in concentrated electrolyte solutions was used to derive new equations for calculation of physicochemical properties of multicomponent systems of electrolyte

solutions: density, specific heat, thermal conductivity, water vapor pressure over solution, activity of water, surface tension, dynamic viscosity coefficient, boiling and freezing points, and electrical conductivity.

(2) New correlation equations were suggested for determining the density of water, specific heat, thermal conductivity, water vapor pressure over solution, dynamic viscosity of water on the saturation line in a wide range of temperatures and pressures. These equations provide the minimum calculation errors.

(3) The physicochemical properties of ammonium sulfate-nitrate solutions were calculated for a mass fraction of the components equal to 10–70% in the temperature range 25–80°C. This made it possible to recommend the equations under consideration for determining these properties for other multicomponent systems of electrolytes as well.

(4) The set of the physicochemical studies performed enabled optimal consideration of heat-and-mass exchange processes that occur in manufacture of a complex integrated fertilizer based on ammonium sulfate and nitrate with addition of microelements from effluent gases of thermal power plants.

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