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## CALCULATED CHARACTERISTIC FOR DESCRIPTION OF ABSORPTION-DESORPTION PROCESSES EQUILIBRIUM IN THE SYSTEMS NH<sub>3</sub> – WATER И SO<sub>2</sub> – WATER

The analysis of existing reference data and the experimental nature of dependencies of the equilibrium conditions for the determination of absorption and desorption processes in the  $NH_3$  – water and  $SO_2$  – water systems was carried out. During reference data processing calculated dependences to the description of equilibrium were obtained. The deviation of the values obtained for the given dependencies of the reference does not exceed 5.4%. Recommendations on the use of dependencies in engineering calculations are given.

**Introduction.** One of the most important stages of the process design of absorption-desorption sets is to define the equilibrium conditions between gaseous and liquid state. It is common thing to express the composition of gaseous and liquid state in this case through interrelated concentrations of absorbed and desorb elements (further – absorbate). Specific meanings of absorbate concentration in the equilibrium conditions depend on its nature, nature of liquid desiccant (absorbent), temperature and pressure.

Concrete values of concentration of absorbate in the conditions of balance depend on its nature, nature of a liquid absorber (absorbent), temperature and pressure. The most simple dependence, described structures of phases in the conditions of balance at absorption (desorption) is the equation of the law of Henry. However for highly soluble gases equilibrium structures can be calculated with sufficient accuracy at application of the law of Henry only at insignificant maintenances of these gases in divided mixes, i.e. by formation of strongly diluted solutions [1].

For definition of equilibrium structures of phases at absorption (desorption) well soluble gases are often used the referenced data received experimental. Such data, as a rule, are presented in a tabular kind. The structure of a gas phase is thus usually presented by values of partial absorbate pressure, and liquid is presented by values of its mass fraction in absorbent at various temperatures. At practical calculations, including computer facilities application, it is inconveniently to use such data. During the calculations necessary for construction of a line of balance of an absorber (desorber), it is necessary to reuse double interpolation: on structure of a phase and on temperature.

To the absorbates, characterized above, concern  $NH_3$  and  $SO_2$  in cases of their interaction with their own water solutions. Adsorption of  $NH_3$  is very widespread stage of carrying out of various technological processes. For absorbation of  $SO_2$  chemisorbents representing water solutions are basically applied. Therefore, for calculations of absorbents for absorption of  $SO_2$  is important the adequate description of a condition of balance in system of  $SO_2$  – water.

**Main part.** The value of equilibrium structures for system  $NH_3$  – water was determined experimentally at the beginning XX. In 1925 T. Shervud carried out the critical review of experimental data selecting the most authentic [2]. These data are listed in fundamental directories [3–6]. Also T. Shervud received the empirical equation for system  $NH_3$  – water [2]:

$$S = Kp^n + 1.27t - 83, \tag{1}$$

where S – weight NH<sub>3</sub>, dissolved in the conditions of uniformity in 1,000 kg of water, kg; K and n – coefficients; p – partial pressure NH<sub>3</sub> over a solution, mm hg; t – temperature, °C.

Rates of coefficients K and n are changing in limits from 0.4 to 1.2 and from 0.5 to 0.8 accordingly depending on temperature and are presented for a range of temperatures from 0 to  $60^{\circ}$ C. Calculations on the equation (1) have shown that satisfactory convergence of calculated data with the experimental is reached only at 40°C. In other cases the relative deviation of ratings from the experimental reaches 15% and more. It is difficult to choose the factors K and n at calculations.

Kovalke, Hougen and Watson [2] received the equation on the basis of thermodynamic data

$$\lg \frac{p}{m} = 7.58 - \frac{1,924}{T},\tag{2}$$

where m – the number of NH<sub>3</sub>, dissolved in 1 kg of water, mol; T – temperature (thermodynamic), K.

The equation (2) gives necessary results at a temperature close to 25°C, and a relative mass

fraction of  $NH_3$  in the solution is not more than 0.068 kg/kg [2].

Devis constructed nomograms on the basis of Shervud's data [2]. The identification of equilibrium data on nomograms is approximately equal to accuracy of the sizes received under the formula (1).

We have attempted to get more exact empirical formulas for the description of balance of system NH<sub>3</sub> – water. To minimize the inaccuracy it is required to use two formula: the first – for values of mass fraction NH<sub>3</sub> in water solution  $\bar{x}_a \leq 0.2$  of NH<sub>3</sub>/kg of a solution:

$$x_{a} = [8,830.79 - 3,389.72 \ln T + 228.226 p_{a}^{*} + + 3.25758(\ln T)^{2} + 1.7643(\ln p_{a}^{*})^{2} - - 44.63071 \ln T \cdot \ln p_{a}^{*}] \cdot 10^{-4};$$
(3)

And the second is for the mass fraction of  $NH_3$  in an aqueous solution of 0.2 to 0.5 kg  $NH_3/kg$  solution:

$$\overline{x}_{a} = [8,691.33 - 1,602.25 \ln T + 5.714 (\ln p_{a}^{*})^{2}] \cdot 10^{-5}, \qquad (4)$$

where  $p_a^* - NH_3$  partial pressure above the solution in equilibrium, Pa.

With the use of dependences (3) and (4) we have carried out the calculations for all values of equilibrium partial pressure  $NH_3$  over its water solutions presented in the directory [4]. Comparison of the referenced and calculated sizes is presented in Table 1 and in Fig. 1.

Table 1 The data on the balance of  $NH_3$  – water at  $t = 19.9^{\circ}C$ 

Partial pressure NH <sub>3</sub> $p_a^*$ , Pa	Relative mass fraction of NH <sub>3</sub> in water solution $\bar{x}_a$ , kg NH <sub>3</sub> /kg water	
	by reference [4]	calculated from (3) and (4)
3,653.03	0.0418	0.0418
6,106.16	0.0650	0.0656
6,132.83	0.0655	0.0658
7,492.72	0.0772	0.0777
10,745.78	0.1015	0,1026
11,505.72	0.1075	0.1078
22,144.85	0.1664	0.1664
28,744.30	0.1940	0.1939
40,316.68	0.2337	0.2330

The relative deviation of ratings from referenced as a whole does not exceed 5%, and at  $x_a > 0.1$  kg

of  $NH_3/kg$  of a solution -1.5%. Thus the root-square deviation makes 0.3%.

Values of equilibrium structures of phases for system  $SO_2$  – water, presented in fundamental directories [2–4, 6, 7], are received and generalized by researchers in 20–50th of the last century. They are given and analyzed in details in the directory [7]. Known calculation dependences for the description of balance of system  $SO_2$  – water are not useable for engineering calculations of absorptive- desabsorptive processes. When processing referenced values from [4] and [7] we have received the following equation:

$$\overline{X}_{SO_2} = [(-3.63 \cdot 10^{-9}t^2 + 3.199 \cdot 10^{-7}t - 8.149 \cdot 10^{-6})p_{SO_2}^* + 6.594 \cdot 10^{-4}t^2 - 7.164 \cdot 10^{-2}t + 2.399]p_{SO_2}^* \cdot 10^{-6}, \quad (5)$$

where  $\bar{X}_{SO_2}$  – relative mass fraction of SO<sub>2</sub> in the aqueous solution, kg SO<sub>2</sub>/kg water;  $p_{SO_2}^*$  – partial pressure of SO<sub>2</sub> above its aqueous solution in equilibrium, Pa.



 over its water solutions in conditions of balance at various temperatures:
 - calculation sizes on the equations (3) and (4);
 o – reference data [4]

Comparison of the calculation and reference sizes describing the balance of system  $SO_2$  – water is resulted in Table 2 and on Fig. 2.

Partial	Relative mass fraction of SO <sub>2</sub> in aqueous	
pressure SO <sub>2</sub>	solution $\overline{X}_{SO_2}$ , kg SO <sub>2</sub> /kg water	
$p^*_{SO_2}$ , Pa	according to [4, 7]	calculated from (5)
3,865.7	0.00497	0.004722
7,864.7	0.0099	0.009510
11,997.0	0.01477	0.014353
16,395.9	0.01902	0.019393
20,928.1	0.02438	0.024460
25,460.3	0.02912	0.029400
30,259.1	0.03381	0.034491
45,055.4	0.04761	0.049293
54,786.3	0.0566	0.058289
64,783.8	0.06542	0.066920
74,914.6	0.07407	0.075035

Table 2 The data on the balance of  $SO_2$  – water at  $t = 20^{\circ}C$ 



Fig. 2. The partial pressure of  $SO_2$  in its aqueous solutions in equilibrium at different temperatures: -- the calculated values from the equation (5)  $\circ$  - reference data [4, 7]

Maximal deviation of calculation values from the reference are approximately about  $\overline{X}_{SO_2} < 0.02$  kg of SO<sub>2</sub>/kg of water. It makes up to 5.4%. A root-square deviation of calculation sizes from reference for all data file makes 1.4%.

**Conclusion.** Dependences (3)–(5) for the description of the balance of absorptive-desabsorptive processes in systems NH<sub>3</sub> – water and SO<sub>2</sub> – water essentially reduce the complexity of calculations in comparison in comparison with application of data in the form of tables and nomograms. In addition, they are adapted for modern system of units of physical sizes SI.

Formulas (3) and (4) give the most accuracy of results than the formulas (1) and (2) and also known nomograms. Such dependences (3)–(5) are recommended for engineering calculations of absorptive-desabsorptive processes in systems  $NH_3$  – water and  $SO_2$  – water.

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