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THERMODYNAMIC MODELING OF OXYGEN DISSOLVATION IN WATER

О.П. Мусов, М.О. Савченко, І.І. Левчук, Л.А. Фролова. Термодинамічне моделювання розчинення кисню у воді. Розглянуто традиційні методи визначення розчинності кисню у воді. Показано їх переваги та недоліки. Відзначено, що особливо великі труднощі виникають при вимірі РК у реальному хімічному процесі, де температура та компоненти системи, а також їх співвідношення змінюються в часі. Запропоновано новий метод визначення розчинності кисню на основі термодинамічного розрахунку рівноважного фазового та компонентного складу системи кисень-вода шляхом мінімізації ізобарно-ізотермічного потенціалу Гіббса за допомогою програмного комплексу «Селектор». Модель заснована на точному рівнянні стану для розрахунку хімічного потенціалу парової фази та хімічного потенціалу рідкої фази. В результаті отримані математичні закономірності розчинення кисню у воді залежно від широкої області температур та тисків, що дозволяє значно полегшити та розширити діапазон достовірного контролю параметрів хіміко-технологічних процесів. Термодинамічна модель дозволяє проводити розрахунки, як у чистій воді, так у кислотних та сольових розчинах, а також з урахуванням парової фази і без неї. Подано рівняння константи Генрі $X_2 = 0.0181P_i \exp(A + B/T + C \ln(T) + DT)$ для кисневого та повітряного середовища від температури в діапазоні 273...373 К та тисків до 10 атм., що дозволяє визначити будь-які проміжні значення. Для цього необхідно в рівняння підставити поточні дані температури та тиску, які легко піддаються виміру. Показано, що в межах цих діапазонів відхилення від експериментальних значень мінімальне ~1%, що дозволяє використання представлених рівнянь у технологічних розрахунках. Визначено значення температури, при якому спостерігається мінімум розчинності кисню, для чистого кисню $T_{\min} = 370.5$ К, для повітря $T_{\min} = 370.3$ К., при цьому значення ентальпії змінює знак.

Ключові слова: Термодинамічне моделювання, Константа рівноваги, кисень, розчинність кисню, ПК «Селектор», Енергія Гіббса

O. Musov, M. Savchenko, I. Levchuk, L. Frolova. Thermodynamic modeling of oxygen dissolution in water. Traditional methods for determining the solubility of oxygen in water are considered. Their advantages and disadvantages are shown. It is noted that especially great difficulties arise when measuring SO in a real chemical process, where the temperature and components of the system, as well as their ratios change over time. The new method for determining the solubility of oxygen based on thermodynamic calculation of the equilibrium phase and component composition of the oxygen-water system by minimizing the isobaric-isothermal potential of Gibbs using the software package "Selector" is proposed. The model is based on the exact equation of state for calculating the chemical potential of the vapor phase and the chemical potential of the liquid phase. The result is mathematical laws of dissolution of oxygen in water depending on a wide range of temperatures and pressures, which allows significantly facilitating and expanding the range of reliable control of the parameters of chemical-technological processes. The thermodynamic model allows calculations to be performed both in pure water and in acid and salt solutions, as well as taking into account the vapor phase and without it. The equation of Henry's constant is given $X_2 = 0.0181P_i \exp(A + B/T + C \ln(T) + DT)$ for oxygen and air from temperatures in the range of 273...373 K and pressures up to 10 atm., which allows determining any intermediate values. To do this, it is necessary to substitute in the equation the current data of temperature and pressure, which are easily measurable. It is shown that within these ranges the deviation from the experimental values is minimal ~1%, which

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allows using of the presented equations in technological calculations. The value of the temperature, at which the minimum solubility of oxygen is being observed, for pure oxygen is determined $T_{\min} = 370.5\text{K}$, for air $T_{\min} = 370.3\text{K}$, the value of enthalpy changes sign.

Keywords: Thermodynamic modeling, Equilibrium constant, oxygen, oxygen solubility, PC "Selector", Gibbs energy

Introduction

A large number of publications indicate a constant interest in the solubility of oxygen (SO) in water. This attention is due to the interest of almost all sectors of the economy:

- the concentration of SO depending on the temperature characterizes the ecological and sanitary condition of water bodies, and also plays a major role in wastewater treatment, as its concentration determines the nature and speed of processes in aeration tanks;

- a similar role of oxygen in water as the most aggressive gas in the processes of electrochemical corrosion of metals. At the same time, it should be noted its dual role. On the one hand, the corrosion rate due to cathodic polarization of the metal increases with increasing oxidant concentration, on the other hand, a passive film is formed on the metal surface, which prevents further corrosion.

This is a non-exhaustive list, where determining the content of the SO is the most important and urgent task. The result is a large number of methods for determining oxygen in water. Conditionally, they can be divided into three categories [1].

Chemicals:

- Winkler's well-known method based on the reaction between $\text{Mn}(\text{OH})_2$ and oxygen in a highly alkaline medium, as well as modified Winkler's methods - iodometric and pyrophosphate;

Physical:

- Manometric method, where the amount of unreacted oxygen is measured by the change in pressure;
- Titrimetric analysis is a quantitative analysis that measures the volume of a reagent of known concentration (titrant) that is expended on reacting with oxygen in solution.

Physico-chemical:

- Laser absorption method based on the absorption of radiation by molecules of the analyte;
- Luminescent method based on the glow of phosphors formed as a result of chemical reactions of oxygen with certain substances;

- Spectroscopic methods are based on selective absorption of light by substances that change the color;

- Electrochemical methods, including amperometric, potentiometric, volt-amperometric, coulometric and conductometric methods;

- Chromatographic methods based on the use of differences in the adsorption of oxygen, other gases and solvent vapors;

- Kinetic method based on measuring the induction period of the oxygen oxidation reaction of ascorbic acid;

- Radiometric methods based on the determination of the radioactivity of elements formed by the interaction of nucleons or radioactive elements with dissolved oxygen;

- Mass spectrometric method is used if the isotopic composition of oxygen is required;

- Resonance methods that use the paramagnetic properties of oxygen. These include the EPR method based on the phenomenon of resonant energy absorption of electromagnetic waves by paramagnetic particles and NMR based on measuring the time (τ) of proton spin-lattice relaxation of paramagnetic particles in solution.

Chemical methods are relatively simple, but they can be implemented only in the presence of a significant amount of chemical reagents. Physical and physico-chemical methods are quite complex, require expensive equipment and highly qualified personnel. Their disadvantages also include the inability of most of them to perform continuous measurements. Of the above methods, only electrochemical are promising because they have a standard electrical output signal and can be used in automation systems. However, they also have significant drawbacks: a small measuring range and they can not provide measurement of SO at temperatures up to 100C and above, in acidic and alkaline environments. In addition, the use of these methods is advisable in the analysis of water in which the temperature and pressure of the environment are relatively constant. Particularly big problems arise when

measuring SO in a real chemical process, where these parameters and their ratios change over time. One example is the technology of obtaining copper sulphate from copper scrap metal. Here, oxygen is the main oxidant, and its concentration is decisive for the impact on the speed of the process as a whole. At the same time, the concentrations of copper sulfate and sulfuric acid in the solution and their ratios are constantly changing, respectively, changing the solubility of oxygen. Thus, the optimization of this process is generally impossible without continuous monitoring of the concentration of SO at different stages of production.

Analysis of publications

The solubility of gases, including oxygen, was determined mainly experimentally and was limited by a narrow temperature range and atmospheric pressure. The most significant are the reviews [1, 2, 3], which provide data both in the form of tables of experimental values and in the form of analytical dependences of SO in water and electrolyte solutions on temperature and partial pressure of oxygen.

In [1] provides data on the solubility of oxygen in water and electrolyte solutions published before 1978. In [2] published the results of the solubility of oxygen in water at a temperature of 273...573 K, as well as in some electrolyte solutions. In [3] the results of oxygen solubility in water and electrolyte solutions up to 1989 are presented and generalized. Experimental methods of studying SO are considered. His view on the cause of the extreme phenomenon of the influence of temperature on the solubility of oxygen.

Later, there were additional data systematized by H.L. Clover [4] and continued by R. Battino [5].

The review [4] provides updated literature data from 1981 to 2010. It is noted a good match of the SO at low pressures, but research is needed at high temperatures and pressures. In addition, a few studies indicate the salt effect of solubility in salt solutions. Indicates the almost complete absence of SO in hydrocarbons and ionic liquids.

This is by no means a complete list of literature on the solubility of gases in water and solutions. The results of these experimental studies are considered the most reliable and were used by us to compare with the obtained values of the SO by calculation.

Experimental problems of measuring SO in water and hydrocarbons are discussed in [5]. The solubility in water is two orders of magnitude lower, so the sensitivity of calorimeters should be 100 times more sensitive to water. This is a big experimental problem.

Thus, there is a need for knowledge of SO under the influence of not only temperature and pressure, but also other indicators that significantly affect the dissolution process (water vapor content in the gas, the presence of salts and acids in the solution).

The aim of the study

The solution to this problem, in our opinion, is a theoretical prediction of the quantitative content of SO in aqueous solution using the methods of thermodynamic modeling. The revealed mathematical regularities of dissolution of oxygen in water depending on temperature, pressure, concentration of various acids and salts will allow to facilitate considerably and expand areas of reliable control of parameters of chemical-technological process.

The purpose of this work is to substantiate the possibility of using, using thermodynamic modeling in water – atmosphere and water – oxygen systems, a theoretical approach to determine the SO in aqueous solution. The adequacy of theoretical and experimental data will allow the use of research results in solving various technological problems of automation and process optimization.

Research methodology

By comparing the chemical potentials of oxygen above the water surface and in its volume, at the equilibrium state of the system ($p, T = \text{const}$) it is possible to obtain the functional dependence of the solubility of the gas in liquids on temperature.

The dissolution of gaseous oxygen in water at equilibrium is described by the equation:



the equilibrium in the system is determined by the equality of the chemical potentials of the gas in the gas μ_1 (J/mol) and liquid μ_2 (J/mol) phases:

$$\mu_1 = \mu_2. \quad (2)$$

Hereinafter, the lower index “1” refers to the gas phase, and the lower index “2” to the solution. The equilibrium constant k of equations (1) and (2) will be determined by the expression:

$$k = \frac{\alpha_2}{f_1}, \quad (3)$$

where f_1 – gas fugitive, and α_2 is the activity of dissolved oxygen.

At gas pressures not exceeding 10 atm and in dilute solutions close to ideal, we can write:

$$\alpha_2 \rightarrow [O_2(aq)], \quad (4)$$

where P_1 – oxygen partial pressure, [atm], $[O_2(aq)]$ – the concentration of dissolved oxygen in the solution [mol/l].

Given (4) equation (3) can be represented as:

$$k = K_H = \frac{[O_2(aq)]}{P_1}, \quad (5)$$

where: K_H – Henry’s temperature-dependent constant $\left[\frac{\text{mol}}{1 \cdot \text{atm}} \right]$.

The chemical potentials of oxygen in the gas phase and in solution can be expressed as follows:

$$\mu_1 - \mu_2^0 = RT \ln P_1, \quad (6)$$

$$\mu_2 - \mu_2^0 = RT \ln [O_2(aq)], \quad (7)$$

where: μ_1^0 – standard chemical potential of oxygen in the gas mixture at its partial pressure is equal to 1 atm;

μ_2^0 – standard chemical potential of oxygen in solution at its concentration equal to 1 mol/l,

R – gas constant (8.3144 J/(mol·K)),

T – absolute temperature, K.

The Gibbs energy of reaction (1) at temperature can be calculated from the equation:

$$\mu_2^0 - \mu_1^0 = -RT \ln k = \Delta G^0. \quad (8)$$

Substituting expression (6), (7) into equation (5), taking into account (6) and (8), and converting it, we can obtain the relation:

$$k = K_H = \frac{[O_2(aq)]}{P_1} = e^{-\frac{\Delta G^0}{RT}}. \quad (9)$$

If we use the data [3], which are considered the most reliable, for the molar fraction of SO in water $X_2 = 2.301E-5$, at 298.15 and oxygen pressure of 1 atm, and convert it into mol/l, then from (9) you can get $\Delta G_{298}^0 = 16524$ J/mol. The low positive Gibbs energy indicates a significant dependence of the equilibrium constant on temperature and pressure.

To calculate the SO in water at different temperatures and pressures in this work by thermodynamic modeling, we calculated the equilibrium phase and component composition of the system by minimizing the isobaric-isothermal Gibbs potential using a software package, then PC, “Selector” [6, 7]. This PC allows the calculation of complete, metastable and intermediate chemical equilibria in systems where aqueous electrolyte solution, gas mixture, liquid and solid one- and multicomponent phases may be present at the same time. “Selector” contains a built-in system of internally agreed thermodynamic databases and a bank of initial chemical compositions.

In this work, pure water was chosen as a simplified liquid phase. In the future it is planned to study SO in acidic and alkaline systems. The gaseous medium was taken as pure oxygen or atmos-

phere with the following relative atomic composition: Ar0.3209C0.01036N53.9478 Ne0.000619O14.48472. Table 1 presents the initial concentrations of components and calculation parameters.

Table 1

Initial concentrations of components and calculation parameters

H ₂ O	Air	O ₂	Pressure	Temperature
mole	mole	mole	atm	K
55.34	10	10	1...10	273.15...573.15

The liquid phase was determined in the amount of 1 l of H₂O and was considered open to the gas phase.

Thermodynamic characteristics, standard Gibbs energy, enthalpy and entropy, formation of compounds from elements and many possible components are taken from the bases of PC “Selector” (a_sprons98.DB and g_sprons98.db).

Accepted assumptions:

- Dissolved oxygen in water in the form of O₂ molecules.
- The tank is closed, ie there is no mass transfer with the environment.
- No oxygen consumption inside the tank by oxidation reactions and the like.
- There are no insoluble mineral components.
- The partial pressure of oxygen was maintained constant.

The Gibbs energy obtained above by formula (9) $\Delta G_{298}^0 = 16524$ J/mol for the aqueous component O₂^{*} is very close to $\Delta G_{298}^0 = 16543$ J/mol from the base a_sprons98.DB. In [5] the review of results of measurement of partial molar enthalpy at dissolution of oxygen in water is presented. The values ΔH_{298}^0 range from – 12020 J/mol to – 12060 J/mol. In a_sprons98.DB the value ΔH_{298}^0 is – 12133.6 J/mol. Such minor differences in the thermodynamic parameters of the key component indicate the admissibility of their use in the calculations of the PC “Selector”.

Results and discussion

To correctly compare the calculated and experimental data of the SO in the water, calculations were previously performed in the program “Selector” at different mass ratios of water/air and water/oxygen. Calculations have shown that the amount of air and oxygen relative to water does not have a significant effect on the results. Therefore, a constant water/air and water/oxygen ratio of 55.34 mol/10 mol, respectively, was used in the subsequent calculations.

One of the factors influencing the reliability of experimental data on the solubility of the gas phase in water is vaporization, the value of which increases sharply with increasing temperature. As a result, the partial pressure of the gas (oxygen) and, accordingly, its solubility decreases. In experimental studies, it is impossible to completely exclude the proportion of saturated vapor, so the LCD is usually determined taking into account the partial pressure of saturated vapor. PC “Selector” allows you to calculate the solubility of oxygen taking into account the vapor phase without it, ie it is practically possible to simulate both real and ideal experimental conditions. In Fig. 1 shows one of the calculation options.

The graph shows that there are differences in the value of the LCD. The solubility of the gas

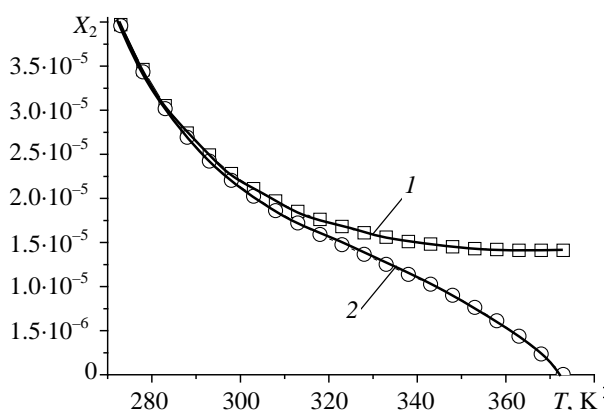


Fig. 1. Influence of saturated steam on SO, $P = 1$ atm:
1 – excluding the vapor phase; 2 – taking into account the vapor phase

without the vapor component decreases monotonically and at 373.15 K the molar fraction of oxygen is $1.42E-5$. Water vapor accounting, which significantly changes the nature of the LCD curve, bringing it to the S – shaped shape. At a temperature of 373.15, the solubility tends to zero. Thus, for a correct comparison of the results of the calculation in the PC and the experimental data, the steam phase was excluded from the calculations.

To compare the calculations in the PC and the results of the empirical equations describing the SO, we used the most qualitative data presented in [1]:

$$\ln X_2 = -66.73538 + 87.47547 / (T / 100K) + 24.45264 \ln(T / 100K), \quad (10)$$

(Average error 0.36% for the temperature range 273-348 K);

in work [1]:

$$\ln X_2 = -3.71814 - 5.59617 * 1e^3 / T + 1.049668 * 1e^6 / T^2, \quad (11)$$

(Average error 0.017% for the temperature range 273-373 K);

in work [3]:

$$\ln X_2 = -54.0411 + 6889.61 / T + 18.554 \ln(T / 100K), \quad (12)$$

(Average error 2.0% for the temperature range 348...573 K),

where: X_2 – molar fraction of dissolved oxygen in water.

The results of calculations of the SO in molar fractions and temperature are shown in Fig. 2.

The figure shows that with increasing temperature, the SO decreases and then increases. The minimum calculated value of oxygen solubility is observed at a temperature of 370.5 K and is $1.4278E-5$. This value of the SO almost coincides with the experimental data presented in [1] – $1.444E-5$ at 373.15 K. It should be noted that the water/oxygen ratio had no effect on the temperature at which the SO is minimal.

The difference in the values of the SO is calculated by the above formulas (10), (11), (12) and thermodynamic calculations are presented in Fig. 3.

As can be seen from the figure, up to 330 K deviations $\&$, according to formulas (10) and (11), have almost the same character and do not exceed 1.7%. However, after 330 K the values according to formula (11) begin to differ significantly and reach – 3.5% at 350 K. Calculations according to formula (12) [5] are similar to the data from (11) [4] in the temperature range 340...373 K. By mistake about 3.5%. Thus, the best coincidence of thermodynamic calculations is observed with the data (2) [5] in the temperature range 273...273 K. The arithmetic mean deviation was 0.7%. Significant discrepancy of the calculation results, at elevated temperatures according to formula (12), may indicate on the one hand, incorrect thermodynamic properties calculated for the compo-

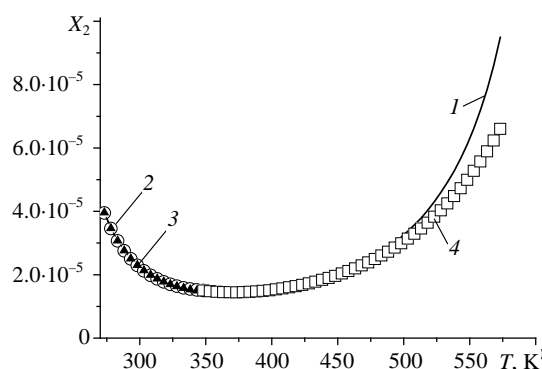


Fig. 2. Dependence of SO concentration on temperature: 1 – calculation in the PC “Selector”, 2 – (10); 3 – (11), 4 – (12)

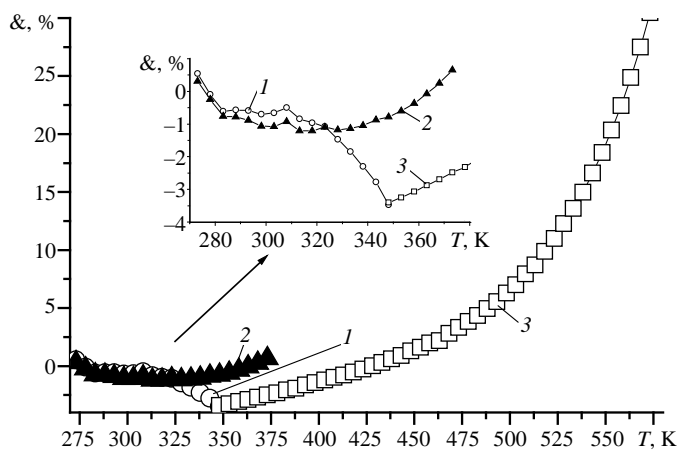


Fig. 3. The relative difference $\&$ % of the values of the SO calculated by the program “Selector” in pure water at $P_{O_2} = 1$ atm from the temperature and by formulas (10), (11), (12)

nents of the aqueous solution by HKF equations in PC “Selector”, on the other hand on measurement inaccuracies due to difficult special conditions during the experiment – 1 atm at normal temperature above 1000 °C. In the future, the calculations will be limited to this temperature, as most of the technological processes that take place at atmospheric pressure do not exceed it.

Given the satisfactory convergence of the results in general, we performed calculations of SO in water-oxygen and water-atmosphere systems at different temperatures and pressures. In Fig. 4 and Fig. 5 present the results. The increase in pressure in both systems leads to a proportional increase in the solubility of oxygen in full accordance with Henry’s law, which applies to ideal systems.

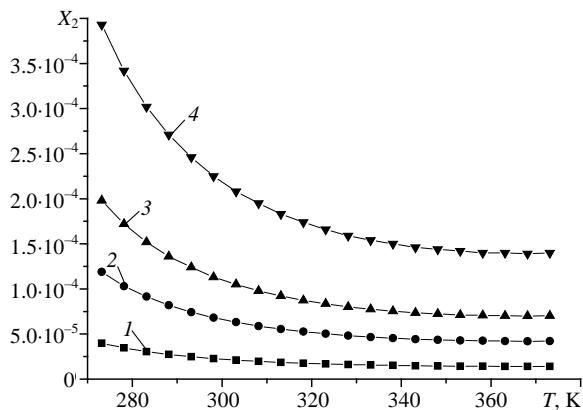


Fig. 4. Dependence of SO on temperature at different pressures O_2 . $C_{H_2O} = 55.34$ mol, $C_{O_2} = 10$ mol :
1 – 1 atm; 2 – 2 atm; 3 – 3 atm; 4 – 4 atm

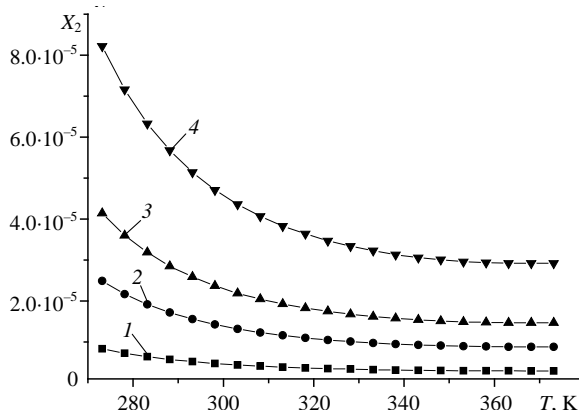


Fig. 5. Dependence of SO on temperature at different atmospheric pressures $C_{H_2O} = 55.34$ mol, $C_{air} = 10$ mol $C_{O_2} = 10$ mol : 1 – 1 atm; 2 – 2 atm; 3 – 3 atm; 4 – 4 atm

The results were processed by Mathcad using the built-in linfit () function in the form of an approximation adopted for gases [8]:

$$\ln K_H = A + \frac{B}{T} + C \ln(T) + DT, \tag{13}$$

where A, B, C and D coefficients Table 2.

$$C_{aq} = P_1 \cdot K_H = P_1 \cdot \exp\left(A + \frac{B}{T} + C \ln(T) + DT\right), \tag{14}$$

with:

$$X_2 = \frac{P_1 \cdot K_H}{M_{H_2O}} = 0.0181 P_1 \exp\left(A + \frac{B}{T} + C \ln(T) + DT\right), \tag{15}$$

where: $M_{H_2O} = 55.34$ mol/l, the number of mol of H_2O in one liter of water at 298.15 K.

The correlation coefficient was $\text{corr}() = 0.9999$.

Table 2

Coefficients of equation (13), (14), (15) to the calculation of SO.
Gaseous medium oxygen/air at 273.15...373.15 K and pressure $P_1 = 1...10$ atm.

Gaseous medium	A	B	C	D
Oxygen	-375.764	14.020e3	59.599	-58.722e-3
Air	-401.139	14.714e3	63.681	-64.668e-3

To find T_{min} with the minimum value of the SO, it is necessary to solve the equation at constant pressure:

$$\frac{\partial X_2}{\partial T} = \frac{P_1}{M_{\text{H}_2\text{O}}} \frac{\partial K_{\text{H}}}{\partial T} = 0, \quad (16)$$

as a result we will receive:

$$RB - RCT - RDT^2 = 0. \quad (17)$$

It is known [5] that at constant pressure:

$$\frac{\partial \Delta G^0 / T}{\partial T} = -\frac{\Delta H^0}{T^2}, \quad (18)$$

where ΔH^0 – molar enthalpy of dissolution of oxygen in water.

Substituting in (18) the expression from (8) we obtain the Gibbs-Helmholtz equation:

$$-RT^2 \frac{\partial \ln K_{\text{H}}}{\partial T} = -\Delta H^0. \quad (19)$$

After differentiation of equation (19) taking into account (13) we can write:

$$-\Delta H^0 = RB - RCT - RDT^2. \quad (20)$$

Comparing (17) and (20) it is obvious that the minimum value of SO corresponds to the change of the enthalpy sign. For pure oxygen $T_{\text{min}} = 370.5$ K, for air $T_{\text{min}} = 370.3$ K.

From the ratio:

$$\Delta G^0 = \Delta H^0 - T\Delta S^0, \quad (21)$$

can be calculated ΔS^0 – the molar entropy of the dissolution of oxygen in water:

$$\Delta S^0 = RA + RC + RC \ln T + 2RDT. \quad (22)$$

Similar results were given in [9, 10], where a thermodynamic analysis of the dependence of SO in pure water and partial pressure of oxygen was performed. However, the equation presented in this paper describes only the oxygen medium without the possibility of taking into account other gaseous and liquid components. PC “Selector”, on the contrary, allows to expand the calculation of equilibrium gas-water systems by including additional source chemical elements.

Conclusions

Despite the large number of methods for instrumental measurement of SO in water, there is currently no reliable and easy way to obtain data at elevated temperatures and pressures. Especially difficulties increase in chemical-technological processes in which these parameters change in time.

The use of PC “Selector” to calculate the equilibrium concentration of oxygen in water revealed the dependence of the Henry constant on temperature and pressure for oxygen and air. The presented equations describing the SO in the temperature range 273...373 K and pressures 1...10 atm, consistent with experimental data with sufficient accuracy ~1% allow to determine any intermediate values. To do this, it is necessary to substitute the current temperature and pressure data into the equation, which are easily measurable. The coincidence of the calculated values of the minimum SO temperature with the experimental data serves as additional confirmation of the adequacy of the calculations. At the same time, it should be borne in mind that the computational experiments do not allow to give unambiguous recommendations for the possible application of equations describing the Henry constant outside these parameters. Such recommendations require additional calculations and comparisons with reliable empirical information.

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