ХИМИЯ

V. F. Nikolaev, A. Kh. Timirgalieva, E. E. Barskaya, D. R. Khanova,
A. V. Egorov, R. B. Sultanova, G. V. Romanov

HYDROGEOCHEMISTRY: NATURAL WATERS IN FULL VIEW

Keywords: natural water, specific refraction, refractive intercept, identification card, oilfield.

A new method has been proposed for identifying the type of natural waters, based on the measurement of the refractive index and the density. Previously, using the data on the refractive indices and densities of the solutions of salts - the macro components of natural waters (chlorides and sulfates of sodium, calcium, magnesium, and sodium bicarbonate), we constructed an identification card (coordinates: refractive intercept - specific Eijkman refraction) on the basis of which it is an easy manner to establish if the test sample of water belongs to a particular type of anion (chloride, sulfate, bicarbonate, mingled), and cation subtype (sodium, calcium, magnesium, combined). The application of a new method of identification of natural waters is demonstrated on the example of the analysis of the samples of oil fields stratal waters, seawater and drinking medicinal-table mineral water.

Ключевые слова: природные воды, удельная рефракция, интерцепт рефракции, идентификационная карта, нефтяное месторождение.

Предложен новый способ для идентификации типа природных вод, основанный на измерении показателя преломления и плотности. Ранее, используя данные о показателях преломления и плотности растворов солей - макро компонентов природных вод (хлориды и сульфаты натрия, кальция, магния, и бикарбоната натрия), построена идентификационная карта (координаты: интерцепт рефракции - удельная рефракция Эйкмана) на основе которой можно простым способом установить, к какому типу принадлежит исследуемый образец по типу аниона (хлорид, сульфат, бикарбонат, смешанное), и подтипу катиона (натрий, кальций, магний, в сочетании). Применение нового метода идентификации природных вод демонстрируется на примере анализа образцов нефтяных месторождений пластовых вод, морской воды и питьевой минеральной лечебно-столовой воды.

Introduction

Total mineralization of natural waters is often determined by the measurement of either density or refractive index. However, simultaneous use of these characteristics of waters allows defining not only the salinity, but the type of natural water.

An important characteristic of natural waters is a mineral composition. Anionic macro components of natural waters, as is known, are the chlorides, sulfates, bicarbonates, and the cationic ones are the ions of the alkali and alkaline earth metals: sodium, potassium, calcium and magnesium. There are different classifications of natural waters on mineral composition. The most widely used classifications were developed by Palmer C.C. (1911) [1], Sulin V.A. (1946) [2] and Piper A.M.(1944) [3]. Graphical representation of the mineral composition of water is considered in [4]. Detailed review of works on the mineral composition of natural waters is given in [5].

Classification of Sulin is based on the genetic principle, according to which the formation of the chemical composition of water occurs in certain natural conditions (continental, marine, depth), and as a result of the interaction of water with rocks or mixing of waters of different origins. According to Sulin there are distinguished the following four main groups of natural waters: sodium sulfate, sodium .bicarbonate, calcium chloride, magnesium chloride. Each type of water according to the predominant anion is divided into three groups - chloride, sulfate and bicarbonate. By predominant cation groups it is divided into subgroups - sodium, calcium and magnesium.

Refracto-densitometric characteristics of solutions

The way for identification of the type of natural waters considered below is very simple. It is based on the two easily identifiable characteristics – refractive index n_D^{20} (further referred to as n), measured at 20ºC on the yellow line of spectrum of the atom Na (the wavelength λ=589 nm), and density d^{20} (further referred to as d), as also defined at 20ºC. The application of this method does not require any serious scientific equipment, except for a portable digital refractometer, working on the yellow LED with the wavelength close to λ≈589 nm) and densitometer (density meter), the total weight of which not exceeding 400-500 g.

As we have shown in the example of evaluating the quality of motor gasoline, valuable information can be obtained by analyzing the position of a point on the fluid sample under study on the refracto-densimetric identification card constructed in the coordinates of refractive intercept and specific refraction [6],[7]. Specific refraction sR is a measure of polarizability per a unit of mass of a matter, which is determined by the electronic structure of ions, atoms and molecules.

The approach realized in [6], in the form somewhat adapted for the analysis of natural waters is not only easy to determine their type, but also easy to visualize the information obtained. This visibility is provided by a combination of two derivatives of the original characteristics of water n and d - refractive intercept RI (1) [8]:

$$RI = n - (d / 2)$$ (1)

with the specific refraction of Lorentz-Lorenz sR_{LL} (2) [9]

$$sR_{LL} = (n^2 - 1) /((n^2 + 2) \cdot d)$$ (2)

with the specific refraction of Gladstone - Dahl (Gladstone – Dale) sR_{GD} (3) [10]

$$sR_{GD} = (n - 1) / d$$ (3)

or with the specific refraction of Eijkman J.F.(1895) (cited by [8])

$$sR_E = (n^2 - 1) /((n + 0,4) \cdot d)$$ (4)

In this study, preference is given to the latter - the specific Eijkman refraction, since in the case of aqueous salt solutions it is additive with a sufficiently high degree of accuracy on mass fractions of components.

Refractive intercept RI of a liquid, being a measure of balance between polarizability and density of matter, possess the additivity property by the volume fractions of components (5) [8], [11]:

$$RI_{MIX} = \sum_{i=1}^{k} RI_i v_i = RI_1 v_1 + RI_2 v_2 + ... + RI_k v_k$$ (5)

Its additivity follows from the additivity of the refractive index of the mixture n_{mix} by the volume fractions of components v_i (6) [9], [12], [13], [14] ($\sum_{i=1}^{k} v_i = 1$)

$$n_{MIX} = \sum_{i=1}^{k} n_i v_i = n_1 v_1 + n_2 v_2 + ... + n_k v_k$$ (6)

and a similar additivity of mixture density d_{MIX} (7):

$$d_{MIX} = \sum_{i=1}^{k} d_i v_i = d_1 v_1 + d_2 v_2 + ... + d_k v_k$$ (7)

where k – number of components in mixture. This rule holds good accuracy both for aqueous solutions, and for hydrocarbon mixtures. Specific refractions are additive on mass fractions of components w_i (8):

$$sR_{MIX} = \sum_{i=1}^{k} sR_i w_i = sR_1 w_1 + sR_2 w_2 + ... + sR_k w_k$$ (8)

It should be noted that the additivity of specific refraction for solutions is performed with much greater accuracy than that of the refractive index n and density d. It should also be noted that if the study uses mass fractions

$$\sum_{i=1}^{k} w_i = 1$$

of components w_i ($\sum_{i=1}^{k} w_i = 1$), then to describe the dependence of the density of the mixture d_{MIX} on the composition there should be used the ratio (9):

$$1 / d_{MIX} = \sum_{i=1}^{k} (w_i / d_i) = w_1 / d_1 + w_2 / d_2 + ... + w_k / d_k$$ (9)

These dependences were obtained under the assumption that the volume of the mixture is equal to the sum of the volumes of the initial components that, with rare exceptions, is done with sufficient accuracy for practical purposes. To construct the identity card of natural water we used the data of the work [15] on the refractive indices n and densities d of aqueous solutions of salts, present in natural waters as macrocomponents – NaCl, CaCl$_2$, MgCl$_2$, Na$_2$SO$_4$, MgSO$_4$, NaHCO$_3$. A large body of data on the refractive indices and densities of the aqueous solutions is given in [16], and on the characteristics of marine waters in [17], [18]. Although in the results of analyzes of natural waters potassium ions are determined as the total with sodium ions, potassium is in most cases a minor component. Its content in the stratal waters of oil

fields makes only 1÷2% of the content of sodium ions. In this regard, solutions potassium salts were not included in our investigation. Basing on the equations (1) and (4) for refractive intercept and specific Eijkman refraction of aqueous salt solutions, the refracto-densimetric card has been constructed (Fig. 1).
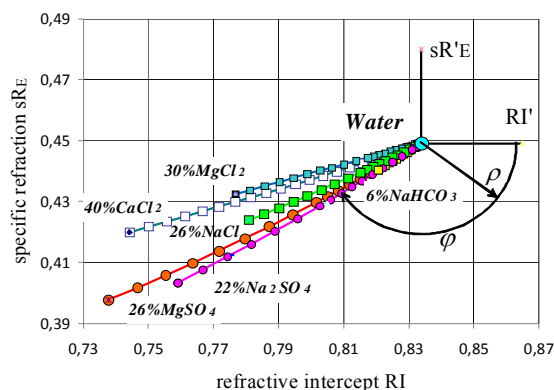

Fig. 1 - Refracto-densitometric card of aqueous solutions of salts in the coordinates of refractive intercept RI – specific Eijkman refraction sR$_E$

It can be seen that the concentrated salt solutions are well differentiated by their location on the card, while the region of low concentration solutions is excessively compressed. If this card was on the smartphone or tablet, you could use a simple stretch or an enlarged scale images. However, for the printed version of the identification card of natural waters this option is inconvenient. In order to provide the same ease of using the card both for highly mineralized water (stratal waters of oil fields), and for the waters of relatively low salinity (curative and table mineral waters), we carried out a double transformation of coordinates "Cartesian coordinates → polar coordinates → Cartesian coordinates", which could be called a "boomerang" transformation. These changes consisted in parallel transition of the Cartesian coordinates to the point "Water" (Fig. 1) and in calculating the new Cartesian coordinates RI' и sR'_E by the ratios (10), (11):

$$RI' = RI - RI_W$$ (10)

$$sR'_E = sR_E - sR_{EW}$$ (11)

where RI_W =0,8339– refractive intercept of water, sR_{EW} = 0.4491 – specific Eijkman refraction for water, followed by calculation of the relations (12) and (13) [18] of the polar angle φ (-180°, 180°) and the radius ρ.

$$\varphi(grad) = 180 \cdot \arctan(RI'/sR'_E) / \pi$$ (12)

$$\rho = \sqrt{(RI')^2 + (sR'_E)^2}$$ (13)

From Tab. 1 it is seen that all salt solutions have negative polar angles. For convenience, it would be possible, of course, by a simple transformation of coordinates to move the concentration dependences to the region of positive polar angles, however, in the positive area there are already aqueous solutions of oxygen-containing organic compounds (sugars, lower alcohols, glycols) and the vast majority of individual organic liquids.

Table 1 - The upper and lower boundaries of the polar angles of salt solutions - macro-components of natural waters in polar coordinates (Fig. 1)

N	Solutions of salts	The boundaries of the polar φ, grad	
		upper	lower
1	Sodium sulfate Na_2SO_4	-145.03	-148.54
2	Calcium sulfate $CaSO_4$	-145.91	-145.91
3	Sodium bicarbonate $NaHCO_3$	-146.62	-147.13
4	Magnesium sulfate $MgSO_4$	-146.97	-151.86
5	Sodium chloride $NaCl$	-151.40	-154.54
6	Calcium chloride $CaCl_2$	-158.74	-161.95
7	Magnesium chloride $MgCl_2$	-163.74	-169.27

Note: The refractive index of saturated aqueous solution $CaSO_4$ (20℃) is determined by the refractometer PAL-RI (Atago, Japan), density - pycnometrically.

Returning to the analysis of Tab. 1, it can be seen that the boundaries of sodium sulfate solutions significantly overlap with the boundaries of solutions of magnesium sulfate and completely cover the boundaries of the polar angles of sodium bicarbonate, and calcium sulfate (point). However, this overlap of intervals can be easily corrected by the transition from the obtained polar coordinates of salt solutions back to Cartesian coordinates, in which already as the abscissa axis there was used not the refraction intercept *RI*, but the polar angle φ, and as the ordinate axis instead of the specific refraction sR_E there serves the polar radius ρ, which is a measure of the remoteness of points from the center of the polar coordinates - point "Water" and simultaneously the measure of mineralization of salt solution (Fig. 2).
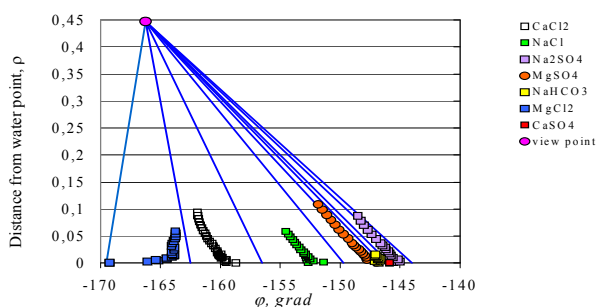

Fig. 2 - Refracto-densimetric card of aqueous solutions of salts (macrocomponents of natural waters) in Cartesian coordinates, using the numerical values of the polar coordinates ρ and φ

A quick glance at Fig. 2 (prior to the application of the points "view point", and the boundary lines of salt solutions) allowed to see in the new coordinates the drive of the points with the growth of ρ (or mineralization) to a certain point or area that can be used as a kind of "observation post" or "view point". A glance from this point to the concentration dependences of the aqueous salt

solutions enables to establish practically non-overlapping boundaries. Coordinates of the "view point" (φ_0; ρ_0) were identified by searching the set of equations of lines passing through both the desired "view point" and the points corresponding to solutions of each salt. As a result of the optimization we obtained the coordinates of the "view point" φ_0=-166.27º: ρ_0=0.44728 and significantly narrowed the boundaries of the polar angles (on the abscissa axis φ at ρ=0), which are cut by straight lines passed through the "view point", and the concentration dependences of the individual salts. Not to confuse the obtained new boundaries of polar angles of solutions with the boundaries of the polar angles of solutions given in Tab. 1, we call them identification polar angles φ_{IPA}. They are given in Table 2.

Table 2 - The boundaries of the identification polar angles φ_{IPA} of aqueous salt solutions using the auxiliary point "view point", the polar radius ρ_{MAX} and the value of mineralization

N	Salt solutions	The boundaries of the identification polar angle of salt solutions φ_{IPA}		Maximum polar radius ρ_{MAX}	Mineralization, g/l at ρ_{MAX}
		upper	lower		
1	Sodium sulfate Na_2SO_4	-144.20	-145.47	0.0878	266.3
2	Calcium sulfate $CaSO_4$	-145.9*	-145.9	0.0011	-
3	Sodium bicarbonate $NaHCO_3$	-146.30	-146.96	0.0160	62.5
4	Magnesium sulfate $MgSO_4$	-146.89	-147.46	0.1090	337.0
5	Sodium chloride $NaCl$	-151.33	-152.77	0.0587	311.3
6	Calcium chloride $CaCl_2$	-158.72	-160.84	0.0944	558.3
7	Magnesium chloride $MgCl_2$	-163.39	-169.28	0.0596	382.9

When analyzing the new boundaries of salt solutions it can be seen that by using coordinate "boomerang" transformations we completely eliminated the overlapping of the boundaries of solutions of sodium sulfate and magnesium sulfate. A slight overlap of the boundaries of the identification polar angles of magnesium sulfate and sodium bicarbonate solutions (~0.07º) is observed in the region of low mineralization. The point of a saturated solution of calcium sulfate is beyond the boundaries of solutions of other salts.

Algorithm for identification of the type of natural waters, and examples of its use

Thus, the algorithm for determining the type of natural water can be reduced to the following sequence of operations:

1. Measurement of refractive index $(n_D^{20})_i$ and density $(d^{20})_i$.

2. Calculation of two characteristics of natural waters - refractive intercept $(RI)_i$ by eq.(1) and specific Eijkman refraction $(sR_E)_i$ by eq.(4). That is

$$RI = n - (d / 2); \quad sR_E = (n^2 - 1)/[(n + 0,4)d]$$

3. A parallel transfer of the center of the Cartesian coordinate system $RI; sR_E$ in a Cartesian coordinate system with the center of "water point" and calculation of new coordinates of the test sample of natural water $(RI')_i; (sR_E')_i$ by eq.(10), (11). That is

$$RI' = RI - RI_W, \quad sR'_E = sR_E - sR_{EW},$$

where RI_W =0.8339 и sR_{EW} =0.4491– refractive intercept and specific refraction of water (20ºC).

4. Transfer of coordinates of the test sample point from Cartesian coordinate system $RI'; sR_E'$ to polar coordinates $(\varphi)_i; (\rho)_i$ by eq. (10) – (13). That is

$$\varphi(\text{grad}) = 180 \cdot \text{ATAN2(RI';sR')}/\pi;$$

$$\rho = \sqrt{(RI')^2 + (sR_E')^2},$$

where ATAN2 – function of arctan in the program Microsoft Excel.

5. Computation of the identification polar angle of the sample $(\varphi_{IPA})_i$ by eq.

$$\varphi_{IPA} = -\varphi_0 - \rho_0(\varphi_0 - \varphi_i)/(\rho_0 - \rho_i),$$

where ρ_0=0.4473; φ_0=-166.27º - coordinates of the "view point".

Attribution of natural water sample to a particular type is determined by the identification card (Fig.3).

On the identification card curves 500-5000 mg-eq/l indicate the degree of mineralization of water. Properties of oilfield stratal waters are given in table 3(see next page). In Fig. 3 to illustrate, the concentration dependence for aqueous solutions of sodium perchlorate are also shown, which as believe, is the salt base of Mars water.

If the identification polar angle of the sample $(\varphi_{IPA})_i$ falls within the boundaries of solutions of any individual salt (Tab. 2 and Fig. 3), the mineralization would be calculated by the equations given in Tab. 4.

In order to enable the readers to assess the suitability of the boundaries of identification polar angles (Tab. 2) and identification card (Fig. 3) on the example of natural waters with the known ionic composition and density, but with unknown refractive index, we offer a simple way of approximate estimation of n_D^{20}. To do this, we need to calculate theoretically from the ionic composition using the data of Tab. 5 and eq. (8), the specific Eijkman refraction of natural water, and knowing additionally the density to calculate according to the equation (4), the refractive index n_D^{20}. Specific Eijkman refractions for ions were calculated by us for concentrated solutions of salts.
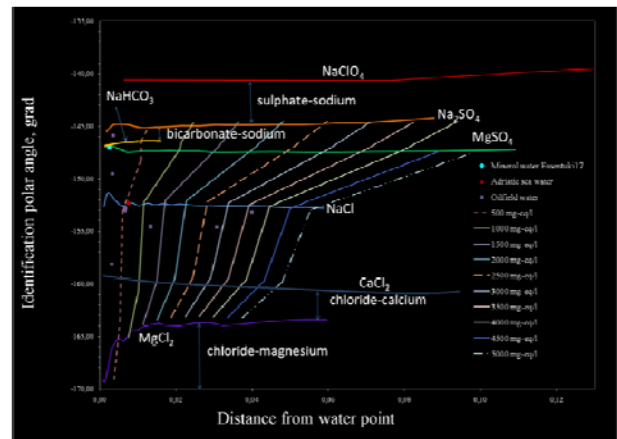

Fig. 3 - Identification refracto-densitometric card for determining the type of natural waters in combined Cartesian - polar coordinates

The experimental value of the specific refraction of water is 0.4491 also indicates the acceptability of the obtained specific refraction of ions.

At the position of the point of natural water in the region of the mixed type, and in the case of presence in it of only two major mineral components (e.g. $CaCl_2$ and NaCl), the ratio between Ca and Na can be estimated by adding to the sample of natural water the solution of one of these components (e.g. NaCl) with the known n_D^{20}, d^{20} and the mass fraction of the component w and measurement n_D^{20}, d^{20} of the obtained mixture. Using the equation (8) you can estimate the ratio of Ca/Na. It should also be noted that the method of identifying the type of natural water can be used when the analyzed waters do not contain the impurities of organic substances. As previously noted, their aqueous solutions in polar coordinates are located in the regions of positive polar angles.

Table 3 - Physico-chemical properties and mineral composition of oilfield waters*

Number of sample	n_D^{20}	d^{20}. g/cm³	Total mineralization. mg/l	Na⁺/K⁺. mg/l	Ca²⁺. mg/l	Mg²⁺. mg/l	HCO₃⁻. mg/l	Cl⁻. mg/l	SO₄²⁻. mg/l	φ_{IPA}	ρ
1	1.3459	1.0470	64546	17060	2665	303.7	579.7	43869.4	44	-154.6	0.01326
2	1.3353	1.0075	16505	5896	120	24.3	2563	7896.5	0	-149.5	0.0033
3	1.3667	1.1320	214028	66599.5	12625.2	2430	280	131608	485	-153.2	0.03997
4	1.3619	1.1330	180531	57551.3	10020	1579.5	256.3	110551	559	-154.6	0.03075
5	1.3389	1.0230	30044	9253	360.7	1233	164.7	16672	2360	-153.0	0.00658
6	1.3390	1.0210	37187	12059	380.8	1202.8	164.7	21059	2320	-152.8	0.00678
7	1.3347	1.0030	10536	3578.4	356.7	94.8	183	6317.2	5	-145.9	0.00355
8	1.3368	1.0090	20322	7100	621.2	111.8	183	12283.4	11	-158.1	0.0032

Note: The refractive indexes are determined by the refractometer PAL-RI (Atago, Japan), density - pycnometrically.
This oilfield waters are the chloride type in Sulin's classification.

Table 4 - The equations for quantitative calculation of water mineralization by the identification polar angle $(\varphi_{IPA})_i$ and the polar radius $(\rho)_i$

Solution of salt	Unit of measurement	The salt content in water	R-squared	Standard Error of Est.
NaCl	mg·eq/l	$= 3064.78 - 1.36633 \cdot 10^6 \cdot \rho + 20.1948 \cdot \varphi - 9540.27 \cdot \rho \cdot \varphi$	99.99	6.62
	g/l	$= 180.193 - 79706.9 \cdot \rho + 1.18733 \cdot \varphi - 556.611 \cdot \rho \cdot \varphi$ $= -51.6288 + 15442.5 \cdot \rho - 0.33935 \cdot \varphi + 98.2047 \cdot \rho \cdot \varphi$	99.99	0.388
	%		99.98	0.113
CaCl₂	mg·eq/l	$= 7348.55 - 697290.0 \cdot \rho + 46.1793 \cdot \varphi - 5002.65 \cdot \rho \cdot \varphi$	99.99	11.20
	g/l	$= 409.885 - 38597.9 \cdot \rho + 2.5759 \cdot \varphi - 277.013 \cdot \rho \cdot \varphi$ $= -250.138 + 12282.3 \cdot \rho - 1.57001 \cdot \varphi + 73.8248 \cdot \rho \cdot \varphi$	99.99	0.619
	%		99.89	0.432
MgCl₂	mg·eq/l	$= -2274.37 - 212293.0 \cdot \rho - 13.5037 \cdot \varphi - 2129.34 \cdot \rho \cdot \varphi$	99.99	17.30
	g/l	$= -107.133 - 10127.7 \cdot \rho - 0.635954 \cdot \varphi - 101.498 \cdot \rho \cdot \varphi$ $= 32.3309 - 11143.3 \cdot \rho + 0.193482 \cdot \varphi - 71.2528 \cdot \rho \cdot \varphi$	99.99	0.821
	%		99.92	0.277
Na2SO4	mg·eq/l	$= -4341.47 + 344080.0 \cdot \rho - 29.8091 \cdot \varphi + 2085.86 \cdot \rho \cdot \varphi$	99.99	9.11
	g/l	$= -316.773 + 24551.8 \cdot \rho - 2.17531 \cdot \varphi + 148.934 \cdot \rho \cdot \varphi$ $= 31.6596 - 2814.33 \cdot \rho + 0.217093 \cdot \varphi - 21.2172 \cdot \rho \cdot \varphi$	99.99	0.643
	%		99.98	0.101
MgSO4	mg·eq/l	$= 12499.5 + 795066.0 \cdot \rho + 85.2522 \cdot \varphi + 5048.38 \cdot \rho \cdot \varphi$	99.99	18.65
	g/l	$= 737.299 + 48077.1 \cdot \rho + 5.02909 \cdot \varphi + 305.373 \cdot \rho \cdot \varphi$ $= -116.045 - 7449.77 \cdot \rho - 0.791006 \cdot \varphi - 52.1949 \cdot \rho \cdot \varphi$	99.99	1.133
	%		99.96	0.160
NaHCO3	mg·eq/l	$= -2790.77 + 21837.3 \cdot \rho - 18.983 \cdot \varphi - 173.811 \cdot \rho \cdot \varphi$	99.99	1.895
	g/l	$= -230.39 + 880.804 \cdot \rho - 1.56694 \cdot \varphi - 21.128 \cdot \rho \cdot \varphi$ $= 1.44235 - 3084.17 \cdot \rho + 0.00990073 \cdot \varphi - 23.6456 \cdot \rho \cdot \varphi$	99.99	0.148
	%		99.99	0.005

Table 5 - Optimized specific Eijkman refractions sR_E for water and ionic macrocomponents of natural waters

Ca^{2+}	Mg^{2+}	Na^+	Cl^-	SO_4^{2-}	HCO_3^-	*Water*
0.1722	0.1068	0.1370	0.4900	0.2868	0.3580	0.4496

Conclusion

The express-method for identification of natural water on bases mineral composition discussed in the work does not require bulky equipment and is characterized by high clarity. It can be used as a methodical support for the manufactured refracto-densitometric analyzers.

References

[1] C.C. Palmer The geochemical interpretation of water analysis. USGS. Bull. 1911; 479: 4-31.

[2] Sulin VA. Basis of classification of natural waters. Moscow, USSR 1946. Russian.

[3] Piper AM. A graphic procedure in the geochemical interpretation of water analyses. Trans. Amer. Geophys. Union. 1944; 25: 914-923.

[4] Abdel-Lattif A. Groundwater chemistry of the shallow aquifer, el-tur area, south Sinai, Egypt. Journal of Environmental Hydrology. 2003; 11(11): 1-16.

[5] Samarina VS. Hydrogeochemistry. (L.: Leningrad State Univ-ty, 1977: 360. Russian.

[6]Nikolaev VF, Tabrisov II, Penkovsky AI, et al. Express method for total content assessment of aromatic hydrocarbons and oxygen in finished gasolines by refractometry and densimetry. Fuel. 2015; 142: 94 – 101.

[7] Nikolaev VF. Rapid methods for testing composite products of oilfield chemistry and motor fuels. Ministry of Educ. and Sci. of Russia: Kazan National Research Technol. Univ-ty – Publish. House: KNITU. 2012: 124. http://dx.doi.org/10.13140/2.1.3427.4566 [ISBN 978-5-7882-1257-9]. Russian.

[8] Kurtz SS. Physical properties and structure of hydrocarbons. In: Brooks BT, Kurtz SS, Boord CE, et al. edit. Chemistry of petroleum hydrocarbons, N-Y. 1954; 1.

[9]Ioffe BV. Refractometric chemistry techniques. (3rd ed. Leningrad: Chemistry. p. 352, 1983). Russian.

[10] Gladstone JH, Dale TP. On the influence of temperature on the refraction of light. Phil. Trans. Roy. Soc. 1858; 148: 887-894.

[11] Heifetz EM. New methods for determining the chemical composition of fuels and oils. (Bureau of technical and economic information TSIMTNEFT – Moscow, Leningrad: GNTI NGTL. 1950: 64. Russian.

[12] NikolaevVF, Sultanova RB, Penkovsky AI, et al. Methods of determining the composition and model description of physical-chemical and performance properties of multicomponent mixtures. Kazan National Research Technol. Univ-ty – Publish. House: KNRTU;. 2008: 180. [ISBN 978-5-7882-0653-0]. Russian.

[13] Nikolaev VF, Tabrisov II, Sultanova RB. Description of physical and chemical properties of the three-component models of commercial gasoline. Herald of Kazan Technol. Univ-ty.2010; 13(10): 342-349. Russian.

[14] Tabrisov II, Iskorkin AD, Sultanova RB, et al. Description and prediction of physico-chemical properties of the pseudo ternary commodity gasoline models based on the data on pseudobinary mixtures. Herald of Kazan Technol. Univ-ty. 2011; 14(10): 143-147. Russian.

[15] Lide DR (editor). Concentrative Properties of Aqueous Solutions: Density, Refractive Index, Freezing Point Depression, and Viscosity, in CRC Handbook of Chemistry and Physics, Internet Version (http://www.hbcpnetbase.com/), Taylor and Francis: Boca Raton, FL. 2006.

[16] International critical Tables of numerical Data, Physics, Chemistry and Technology, McGRAW-HILL BOOK Company, Inc., 1930; VII.

[17] Austin RW, Halikas G. The index of refraction of seawater, SIO Ref. No. 76-1, Scripps Inst. Oceanogr., La Jolla, 1976: 121.

[18] Morel A. Optical properties of pure water and pure seawater. in Jerlov NG, Steeman E. eds. (Academic) Optical Aspects of Oceanography,. 1974: 1–24.

© **В. Ф. Николаев** - д-р хим. наук, ИОФХ им А.Е. Арбузова КазНЦ РАН, Казанский национальный исследовательский технологический университет, mobin7@yandex.ru; **А. Х. Тимиргалиева -** студент КНИТУ, timirgalieva94@mail.ru; **Е. Е. Барская** - канд. хим. наук, ИОФХ им А.Е. Арбузова КазНЦ РАН; **Д. Р. Ханова** - студент КНИТУ; **А. В. Егоров** - канд. хим. наук, ООО Налко Чемпион, Казань, Россия; **Р. Б. Султанова** - канд. хим. наук, доцент кафедры ТООНС КНИТУ; **Г. В. Романов** - д-р хим. наук, ИОФХ им А.Е. Арбузова КазНЦ РАН.

© **V. F. Nikolaev**, Dr.Chem.Sci., A.E. Arbuzov Institute of organic and physical chemistry Kazan Scientific Center of Russian Academy of Sciences, Kazan national research technological university, mobin7@yandex.ru; **A. Kh. Timirgalieva**, student, Kazan national research technological university, timirgalieva94@mail.ru; **E. E. Barskaya**, PhD, A.E. Arbuzov Institute of organic and physical chemistry Kazan Scientific Center of Russian Academy of Sciences; **D. R. Khanova**, student, Kazan national research technological university; **A. V. Egorov**, LLC Nalco Champion, Kazan, Russia; **R. B. Sultanova**, PhD, docent Department Technology of basic organic and petrochemical synthesis, Kazan national research technological university; **G. V. Romanov**, Dr.Chem.Sci., A.E. Arbuzov Institute of organic and physical chemistry Kazan Scientific Center of Russian Academy of Sciences.