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PHENOMENOLOGICAL MODEL OF SPATIAL DISTRIBUTION OF WATER MOLECULES UNDER NORMAL CONDITIONS OR IN A SUPERCRITICAL STATE

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The paper provides a brief description of the results of studies of the properties of water under normal conditions or in a supercritical state. The configuration of the electron shells of a water molecule under normal conditions is described. It is proposed to consider the distribution of molecular spheres (MS) of water as dense layered packings that quickly replace each other during their sedentary arrangement. It is shown that the proposed description of the MS distribution corresponds to the pair correlation function of water under normal conditions or in a supercritical state.

INTRODUCTION

Water is the most common natural resource on Earth, having many applications due to its physical, chemical and biological properties. In nuclear power engineering, the study of the properties of supercritical (SC) water for use as a coolant in IV generation nuclear reactors has a scientific and practical interest [1–4]. According to reference data, water is in a supercritical state when its pressure and temperature exceed the critical ones: $T_c \approx 646.9$ K, $P_c \approx 22.060$ MPa.

Water in the SC state is not only a good heat carrier, but also a good solvent. A large number of works are devoted to the study of its dissolving properties. For example, in [2], experimental data were obtained on the corrosion resistance of 12X18H10T austenitic steel samples under mechanical stress and irradiation with accelerated electrons after 500-h exposure in situ in a SC water convection loop. The effect of the absorbed dose and the level of mechanical stress on their general irradiation-induced corrosion was revealed. The composition and microstructure of the corroded surface are discussed with emphasis on the effects of irradiation and stress on the stability of the protective coating, intergranular corrosion and the occurrence of crack precursors.

Despite the widespread practical application of water in the supercritical state, there is no established physical model in the scientific literature that explains the molecular structure and high dissolving power of liquid and supercritical water. Therefore, there are ongoing discussions in this direction and the search for approaches to describing the structure of liquid and supercritical water continues. For example, in [5], a new approach to describing the structure of liquid and supercritical water is proposed, based on the concept of energetically preferable short-range order variations. The validity of the proposed concept was tested on phenomena that are still unclear but are observed during the transition of liquid water to a supercritical state. The authors concluded that the supercritical state of a substance is a special state to which the concept of "liquid-like" is hardly applicable at high pressures. In a physical sense, this is most likely a microheterogeneous mixture of "gas-like" and "liquid-like" configurations of molecules, rapidly replacing each other. The authors of the article note its controversial nature, although, in their opinion, the article can initiate a useful scientific discussion.

In [6], the dynamics of water molecules in the sub- and supercritical states were studied using inelastic X-ray scattering and numerical modeling. It was shown that with increasing temperature, the network of hydrogen bonds decreases and the spectral weight shifts from HF to LF, which leads to a transition from "liquid-like" to "gas-like" dynamics with rapid changes around the Widom line. The studies showed that hydrogen bonds in water do not disappear with increasing temperature, but only undergo quantitative changes towards a decrease. It was shown that near the supercritical point, where the density of water is very low, small clusters predominate, mainly dimers and trimers, but many molecules do not have hydrogen bonds. However, in SC water, because of a change in the number of hydrogen bonds with increasing temperature and pressure, it is possible to form not only small clusters (dimers and trimers), but nanoclusters, which are formed because of the redistribution of chemical bonds. For example, in work [7] a model for the formation of large-sized nanoclusters of various configurations (flat or volumetric) in carbon dioxide in the SC state was proposed.

However, the studies described above rely on numerical models for calculating various cluster formation variants and do not rely on a physically based model of the molecular structure of water under normal conditions or in the supercritical state.

The purpose of this article is to generalize existing models and propose a new model for the structure of water in the normal and supercritical states.

1. CONFIGURATION OF ELECTRONIC SHELLS OF WATER MOLECULES UNDER NORMAL CONDITIONS

It is known that the spatial configuration of the atoms of a water molecule in an equilibrium state is described by an isosceles triangle, at the apex of which is an oxygen atom, and at the apexes of the angles at the base are hydrogen atoms [8–10].

The length of the bond between the hydrogen and oxygen atoms H – O is $l_{\mathrm{H-O}} = 0.9584$ [9], 0.957 Å [10], the angle at the oxygen atom is 104.5° [9], the length of the bond between the hydrogen atoms is $l_{\mathrm{H-H}} = 1.5$ Å [9], 1.54 Å [10], the height of the isosceles triangular molecule $\mathrm{H_2O}$ is $h_{\mathrm{H_2O}} = 0.59925$ Å.

The electron shells of the water molecule are in the volume of a regular tetrahedron [8], as shown schematically in Fig. 1. The length of the edge of a tetrahedron is equal to the length of the bond between hydrogen atoms $l_{\mathrm{H-H}}$, and the tetrahedron itself is inscribed in a sphere with radius $R_{\mathrm{H_2O}} \equiv r_0 = (\sqrt{6}/4) l_{\mathrm{H-H}} \approx 0.92 \ldots 0.94$ Å [11].

Based on the Pauli principle [8], the electron shells should be maximally distant from each other and indistinguishable, which corresponds to their symmetrical arrangement inside the tetrahedron. Symmetrical arrangement of the electron shells is observed when the center of the O′ sphere and the oxygen atom O are at 0.532634 and 0.59925 Å from the $l_{\mathrm{H-H}}$ bond, respectively. These distances are measured along the line h passing through the center of the sphere and connecting the midpoints of the opposite sides of the tetrahedron (Fig. 2). In this case, the distance between the center of the O′ sphere and the oxygen atom O is $h_O - h_{O'} = 0.06658$ Å.

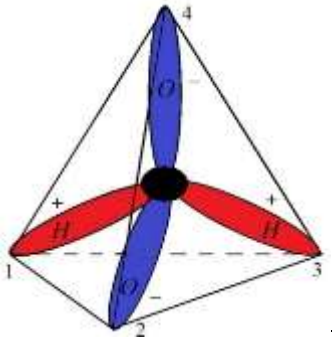

Fig. 1. The arrangement of electron shells of a water molecule in a regular tetrahedron

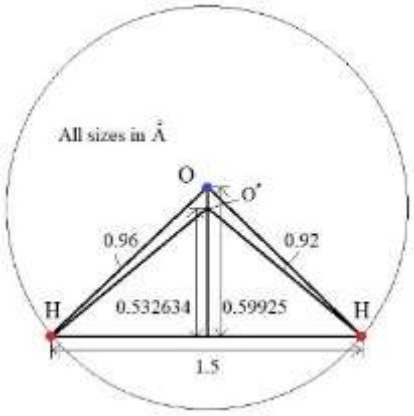

Fig. 2. Distances in a water molecule located in a sphere of radius R_{H_2O}, in a section by the plane of the water molecule

In scientific literature, a sphere with an effective radius of $R_{\mathrm{H_2O}}$ is not used as a water molecule, but a sphere with a radius of $R_0 \approx 1.38$ Å [12–14], 1.35 Å [15], or 1.25 Å (Van Arkel and de Boer molecule) [16].

Therefore, for the sake of certainty, in further calculations we will model the water molecule as a sphere with a radius of $R_0 = 1.38$ Å, which we will call the molecular sphere (MS).

Fig. 3 shows a schematic representation of the MS structure.

In addition to the above-mentioned geometric dimensions of MS, it should be added that its dipole moment is directed along the height of the water molecule from the oxygen atom to the base and is equal to $d_{\mathrm{H_2O}} = 1.86$ D [10] or $d_{\mathrm{H_2O}} = 1.85$ D [16].

It follows from the geometric constructions that the dipole moment vector passes through the center of MS, and the center of gravity of the water molecule coincides with the geometric center of MS. The latter circumstance is important when considering the rotational degrees of freedom, since the orientation of the dipole moment vector will not change to the opposite one, caused by the effect of the "Chinese" spinning top [17].

In addition to the dipole moment, MS has another characteristic, which is spin isomerism (SI). SI characterizes the ability of the water molecule to exist in two forms that differ in the orientation of the nuclear spins of the hydrogen protons [18]. Spins of protons can be oriented either in one direction (ortho-molecule, has a magnetic moment) or in the opposite direction (para-molecule, no magnetic moment). Water in the form of vapor consists of three-quarters ortho-molecules and one-quarter para-molecules, i.e. the ratio ortho/para (O/P) in the vapor phase is 3:1. Moreover, mutual transformations of ortho- and para-molecules are unlikely.

Thus, in further study we will model the water molecule as MS with radius $R_0 = 1.38$ Å with a dipole moment equal to the dipole moment of the water molecule $d_{\mathrm{H_2O}} = 1.86$, with the center of gravity coinciding with the center of MS.

The term water structure can be understood as one of the definitions of Ya. Frenkel [19].

However, in our opinion, another approach is more realistic, describing the structure of water as an infinite set of all possible molecular configurations [20], which arise because of local fluctuations of thermodynamic parameters. This conclusion is based on the fact that when moving, water molecules tend to adopt configurations that correspond to the minimum of free energy in the local volume. Such configurations in the

energy dimension are more favorable and, therefore, arise more often or exist longer.

When considering various configurations of water molecules, the minimum energy is possessed by configurations in the form of dense packings MS. In this case, the energy of electrostatic interaction of electron shells MS, as well as the energy of their dipole-dipole (d-d) and spin-spin (s-s) interactions contribute to the energy of water molecule configurations. Calculations show that d-d interaction can lead to the sphere r_0 shifting relative to the center of MS without going beyond its limits. In this case, the energy of s-s interaction is significantly less than the energy of d-d interaction, and it can be ignored.

2. DISTRIBUTION OF WATER MOLECULES IN SPACE UNDER NORMAL CONDITIONS

Let us estimate the average distance between MS under normal conditions (NC) and compare the obtained result with the characteristic distances of the pair correlation function of water [5].

At present, there is a point of view that the most preferable molecular configuration of the distribution of water molecules corresponds to a regular tetrahedron, in which the distance between the molecules located at the vertices of the tetrahedron and the central molecule is 2.8 Å, and the distance between the molecules at the vertices of the tetrahedron is 4.5 Å [5].

However, such a spatial configuration violates the condition of equidistance of water molecules in the equilibrium state. Therefore, it is necessary to continue searching for such a distribution of water molecules in space that ensures their equidistance.

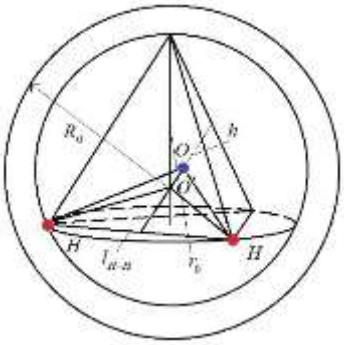

Fig. 3. Schematic diagram of the structure of MS. Sphere R_0 with center O´ and a regular tetrahedron inscribed in the sphere r_0

In the monomolecular layer of water with the densest packing MS, the distance between the MS centers is 2.76 Å. This distance corresponds to the first maximum of the pair correlation function of water $g(r)$ (Fig. 5), which is achieved at the correlation radius $l_{H_2O}^{(0)} \approx 2.8$ Å [5]. The next question is the distribution of water molecules relative to the layer of water with the densest packing MS.

Below, we will adhere to the assumption of Ya. Frenkel [21] that in liquid bodies, atoms do not remain bound for a long time in the same equilibrium positions. From time to time, they jump from one position to the neighboring one. The time of this equilibrium sedentary position τ is greater, the lower the temperature of the liquid. Thus, liquids during such a settled position can be considered as solids, except for a small number of disordered particles, which can be considered as defects. For example, the settled position MS of water at NC is estimated by the value $\tau \approx 1.9 \ldots 10^{-12}$ s, which is significantly greater than the characteristic period of oscillations performed by an ion of the crystal lattice around its temporary equilibrium position $\tau_0 \approx 10^{-13}$ s, located in the same conditions.

2.1. MS DISTRIBUTION IN DENSE LAYER PACKING

During the time of the settled arrangement, we will consider filling a certain volume of water with the densest packing MS. Such filling can be represented as a layer-by-layer arrangement from bottom to top of dense monomolecular layers of water MS in the volume. In this case, we assume that in the equilibrium state, MS are not deformed, but only touch [22].

2.2. MONOMOLECULAR LAYER WITH THE DENSIEST PACKING MS

The densest packing of the MS layer with thickness $2R_0$ is observed when the MS are inscribed in regular hexagonal right prisms (Fig. 4) with height $2R_0$ and side length $2R_0/\sqrt{3}$. Hexagonal right prisms completely fill the volume of the molecular layer.

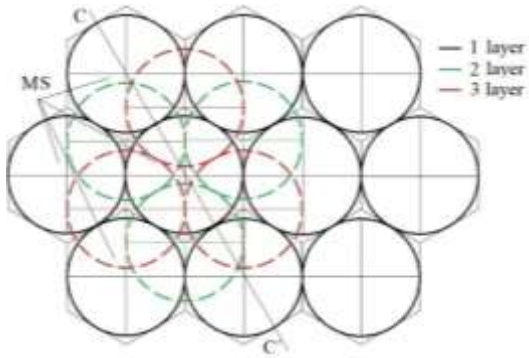

Fig. 4. The arrangement of MS in the molecular layer (top view) with the densest packing (black solid lines)

2.3. SECOND AND SUBSEQUENT MONOMOLECULAR LAYERS WITH THE DENSIEST PACKING MS

The second monomolecular layer with the densest packing of MS is located above the first, as shown in Fig. 4 (green circles). With the densest packing, MS of the second layer should be located in the depressions formed by three adjacent MS of the first layer. It follows from Fig. 4 that MS of the second layer do not fill all the depressions – one of the two adjacent depressions always remains free. In the third layer, MS can be stacked in two ways.

The first packing method is called hexagonal close-packed (HCP). To form HCP, it is necessary to arrange MS of the third layer so that they are in the same positions as in the first layer (the black circles of the first and third layers coincide). For subsequent layers, the order of MS arrangement is repeated (the fourth layer repeats the second, the fifth repeats the third, etc.).

The second packing method is called face-centered cubic (FCC), or cubic close-packed. To form HCP, it is necessary to arrange the MS of the third layer so that they are located above the depressions of the first layer, which the MS of the second layer left free (red circles). Fig. 4 shows HCP MS involving four layers, where the MS of the fourth layer repeat the positions of the MS of the first layer.

In HCP and FCC, the densest packings of MS, the number of nearest neighbors is 12, and the fraction of the volume occupied by MS (packing density) is about 74% [23]. The distance between MS, as in the first molecular layer, will be about 2.8 Å.

HCP and FCC packings contribute to the pair correlation function in the form of the first maximum of the pair correlation function of water $g(r)$ (see Fig. 5). This maximum is achieved at a correlation radius of $l_{H_2O}^{(0)} \approx 2.8$ Å.

However, the HCP or FCC packings of water are not the only possible ones. In the bulk of water, MS can contact the walls of the vessel and form a boundary surface layer of MS. The boundary surface layer of MS is located between the wall and the first layer of MS of the HCP or FCC packing of water and coincides in contour with layer 1 in Fig. 4. Therefore, MS near the wall are in a different position compared to their position in the bulk, and have a lower packing density than that of HCP or FCC.

It can be assumed that HCP or FCC packings can be present in the bulk of water simultaneously, but at the same time be separated by monomolecular layers common to HCP or FCC packings. In this case, we should talk about a mixed HCP and FCC densest packing of MS, replacing each other during their settled position.

The applicability of this assumption is discussed in [5], where the transition of liquid water to the SC state is considered. According to the authors of the cited article, the state of water is a rapidly changing microheterogeneous mixture of "gas-like" and "liquid-like" MS configurations.

In this case, in the volume of water, due to the presence of a surface film of air, and possibly steam [24] bubbles, there may be surface layers MS, similar to the boundary surface layer MS 1 layer in Fig. 4. This assumption is valid, since, for example, the sizes of stationary air bubbles can significantly exceed the radius MS and be of the order of 200…3000 [25] or 20…10^4 Å [26, 27].

Thus, for bubble radii larger than MS, the surface layers can be considered flat.

Based on the above data, in the following consideration we assume that the bubble size corresponds to the nanorange.

In addition, such nanobubbles have a negative charge [28], the value of which varies in the range of 10^{-17}…10^{-13} C [26]. Below we will discuss the consequences arising from the presence of a monomolecular layer of water with the densest packing of MS between the HCP or FCC packings of monomolecular layers.

3. BOUNDARY SURFACE LAYER MS

Let us consider the variant of close packing of MS near the boundary of the volume. In the vertical section along the line CC′ (see Fig. 4) MS are located one under the other, as shown in Fig. 6. With this arrangement of MS, the electrostatic repulsion of polarization charges has a predominant effect. In this case, the direction of the dipoles is determined by the requirement of the minimum potential energy of the dipole-dipole interaction. This requirement leads to the fact that the dipole vectors $\vec{d}_1$ must be unidirectional and parallel to the vector of the distance between them. This follows from the fact that in the specified orientation the dipoles have a minimum potential energy $U_{min} = -2d_1^2/r^3$ [29], where r is the distance between the dipoles. In this orientation, the dipole moment vectors $\vec{d}_1$ have a direction from the negative charge to the positive one, i.e. it is directed toward the oxygen atom, perpendicular to the base of the triangle *H* - *H* Fig. 2.

Thus, spheres of radius r_0 in the boundary surface layer MS will be repelled from the surrounding mass MS due to the repulsion of the electron shells of water molecules (see Fig. 1), and the dipole moments are parallel to the radius vector between the dipoles.

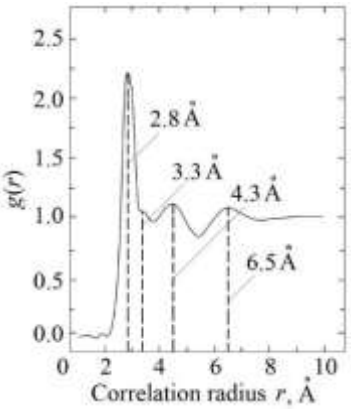

Fig. 5. Dependence of the pair correlation function of water $g(r)$ on the correlation radius r at NC

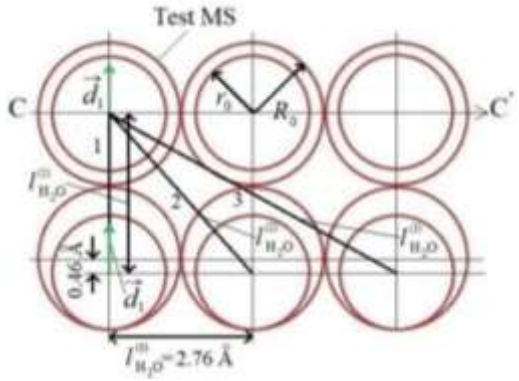

Fig. 6. Location of MS in the first layer (line CC′) and in the boundary layer (layer below line CC′)

Two MS (see Fig. 6) with parallel and unidirectional vectors of dipole moments form a bifurcation dimer (BD) of water $[H_2O]_2$ [30, 31]. The configuration of the formed BD and its characteristic parameters are shown in Fig. 7 [32]. The orientation of the dipole moments of the BD is such that the charge of the surface layer is created by the electron shells of oxygen atoms and therefore has a negative charge. As noted above, the charge of air nanobubbles in water varies in the range of 10^{-17} ... 10^{-13} C [26]. In what follows, we will assume that in the case of vapor nanobubbles, the charge value will be of the same order.

4. ANALYSIS OF THE MAXIMUMS OF THE PAIR CORRELATION FUNCTION OF WATER UNDER NC

The maximum of the water correlation function $g(r)$ can be described based on the geometric constructions of Fig. 6. The first peak of the pair correlation function $g(r)$ at $l_{H_2O}^{(0)} \approx 2.8$ Å is obtained as a result of the above calculation to estimate the distance between water molecules based on their HCP and FCC packing (the densest packing of MS).

The following maxima of the pair correlation function $g(r)$ can be obtained from the estimates following from the location of MS in Fig. 6.

The maximum of $g(r)$ at $r \approx 3.3$ Å corresponds to the distance from the test MS to MS in the boundary surface layer along segment 1:

$$l_{H_2O}^{(1)} = 2.8 \text{ Å} + 0.46 \text{ Å} = 3.26 \text{ Å} \approx 3.3 \text{ Å}. \quad (1)$$

The maximum $g(r)$ at $r = 4.3$ Å corresponds to the distance from the test MS to the MS in the boundary surface layer along segment 2:

$$l_{H_2O}^{(2)} = \sqrt{(3.3 \text{ Å})^2 + (2.8 \text{ Å})^2} \approx 4.3 \text{ Å}. \quad (2)$$

The maximum $g(r)$ at $r \approx 6.5$ Å corresponds to the distance from the test MS to the MS in the boundary surface layer along segment 3:

$$l_{H_2O}^{(3)} = \sqrt{(3.3 \text{ Å})^2 + (5.6 \text{ Å})^2} = 6.5 \text{ Å}. \quad (3)$$

As we can see, the maxima of the pair correlation function $g(r)$ are described by the location of the test MS from the HCP or FCC packings relative to the MS in the boundary surface layer.

Let us now estimate the distance from the test MS to the MS located in the volume of the HCP or FCC packings.

The distance from the test MS to the MS of the second and third rows of HCP or FCC packings, as follows from Fig. 8, are estimated at ~ 4.85 and ~ 5.6 Å, respectively.

The results of the estimates show that the distances from the test MS to the MS of the second and third rows of HCP or FCC packings and in the boundary layer are of the same order. Therefore, the maxima of the pair correlation function $g(r)$ overlap and form a maximum half-width greater than the first maximum half-width.

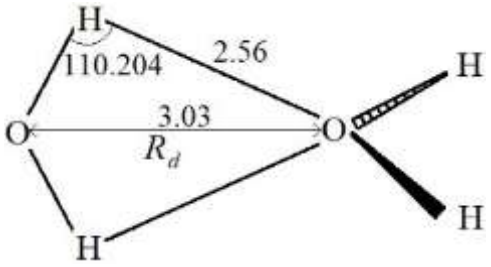

Fig. 7. Configuration of the water BD (all dimensions in Å)

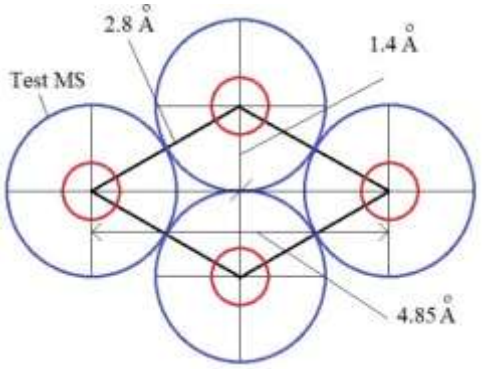

Fig. 8. Distance from the test MS to the MS of the second row of HCP or FCC packages (layer 1, Fig. 4)

Thus, the model of water molecule distribution based on the analysis of the pair correlation function of water $g(r)$ can be formulated by the following statements:

1. In the equilibrium state, MS are grouped into HCP and FCC packings, which can be present in the bulk of water simultaneously and quickly replace each other.

2. In the bulk of water, MS can contact the walls of the vessel and form a boundary surface layer of MS. This boundary surface layer of MS is a monomolecular layer of water with the densest packing of MS, where the distance between the centers of MS is about 2.8 Å.

3. In the bulk of water, due to the presence of a surface film of equilibrium air bubbles or vapor bubbles, surface layers of MS similar to the boundary surface layer of MS can also be present.

4. The distances from the test MS to the MS of the second and third rows of HCP or FCC packings in the boundary layer are of the same order. Therefore, maximums of the pair correlation function are superimposed and, due to incomplete coincidence, are blurred and form a half-width that is greater than the half-width of the first maximum.

5. CHANGE OF MAXIMUMS OF WATER PAIR CORRELATION FUNCTION IN SC STATE

When passing to the SC state, with increasing pressure, the properties of liquid water change in the same way as with increasing temperature [33]. Therefore, let us consider the change in the pair correlation function with an increase in pressure from 1 to 770 MPa. An analysis of such a change shows that the maxima of the correlation function change insignificantly, and their distance to the first maximum decreases. For example, the maxima of the correlation function for 100 to 300 MPa are less than the maximum for 1 MPa, which corresponds to a decrease in short-range order particles. On the other hand, the shoulder maximum at 3.3 increases with increasing pressure. This indicates an increase in the number of particles of a given distance from the test one. This location of the shoulder at 3.3 Å relative to the main maximum at 2.8 Å is typical for substances with loose packing in the solid state [33]. This feature most likely reflects the fact that the liquid partially inherits the structure of the solid after melting.

Thus, from the radial distribution functions of water molecules [33] it follows that when water passes into the supercritical state, a decrease in the distance between the nearest molecules is observed. And considering that surface films are present in the volume of water (conclusion 3 of the previous section), it is possible to remove the controversial characteristic of the question of defining the supercritical state of water [5], and define it as formulated above: a rapidly replacing one another microheterogeneous mixture of "gas-like" and "liquid-like" configurations of molecules.

CONCLUSIONS

The paper provides a brief description of the results of studies of water properties under normal conditions and in a supercritical state. For a general idea, a description of the configuration of the electron shells of a water molecule under normal conditions is given. A description of the arrangement of water molecules in space under normal conditions is proposed, where the concept of molecular spheres (MS) of water is introduced, and their spatial distribution is discussed in the form of dense layered packings replacing each other during their settled position. The distribution in space MS is proposed to be considered as a sequence of monomolecular layers MS, between which a separating layer similar to the boundary surface layer MS can be located. It is shown that the distribution MS proposed for consideration corresponds to the pair correlation function of water under normal conditions or in a supercritical state.

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ФЕНОМЕНОЛОГІЧНА МОДЕЛЬ ПРОСТОРОВОГО РОЗПОДІЛУ МОЛЕКУЛ ВОДИ ЗА НОРМАЛЬНИХ УМОВ АБО В НАДКРИТИЧНОМУ СТАНІ

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Надано короткий опис результатів досліджень властивостей води за нормальних умов або в надкритичному стані. Описано конфігурацію електронних оболонок молекули води за нормальних умов. Розподіл молекулярних сфер (МС) води пропонується розглядати як щільні шаруваті упаковки, які швидко змінюють одна одну під час свого малорухливого розташування. Показано, що запропонований опис розподілу МС відповідає парній кореляційній функції води за нормальних умов або в надкритичному стані.