EQUATION OF STATE FOR METALLIC HYDROGEN AND ATOMIC HELIUM AND THE INTERIOR OF JUPITER AND SATURN

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An equation of state for a mixture of metallic hydrogen and atomic helium has been proposed. The explored intervals of pressure, temperature, and density correspond to the conditions on the largest solar system planets, Jupiter and Saturn. The substance of a planet is modelled as a mixture of protons, helium atoms, and electrons. A theory, where the electron-proton and electron-atom interactions are considered as a perturbation, has been used to find the pressure in the mixture. The electron subsystem is analyzed in the random phase approximation, and the proton-proton, atom-atom, and proton-atom interactions in the hard-sphere approximation. The applicability of the polytropic sphere model for the simulation of Jupiter's and Saturn's internal structures has been analyzed, and a specific value for the polytropic index has been proposed. The density, pressure, and temperature on Jupiter and Saturn as functions of the distance from the planet center have been found. Possible fractions of hydrogen and helium in the planet composition have been estimated.

1. Introduction

After hydrogen in the metallic state under a pressure of 1.4 Mbar and a temperature of 3000 K has been discovered [1, 2] and its properties under terrestrial conditions have been experimentally studied in detail, there appeared a real possibility to research its property under such conditions that nowadays cannot be reproduced on the Earth. From this point of view, giant planets can be regarded as natural laboratories. Owing to the available models for such planets [3–6], we know a number of their thermodynamic characteristics such as the density, pressure, and temperature, as well as their dependences on the distance reckoned from the planet center. All the models are based on the mechanical equilibrium equation for a planet and the polytrope equation. They are known for rather a long time [7, 8]. However, a key characteristic of the substance, which plays a basic role when calculating the density, pressure, and temperature, is the equation of state. Note that, when obtaining metallic hydrogen under terrestrial conditions, only one of three parameters – pressure, density, and temperature – namely, pressure, was measured [1, 2]. Concerning giant planets, we may assert that none of those characteristics can be measured in the central part of the planet. Today, the equilibrium properties of metallic hydrogen are widely studied [9–11], including its equation of state [12–14]. Every improving correction to the equation of state allows the whole set of thermodynamic characteristics of the planet to be calculated more precisely, and the initial model of the planet, which is based on the polytrope equation as well, to be made more specific.

This work aims at studying the equation of state for a mixture of metallic hydrogen and atomic helium in the density and temperature ranges that are characteristic of giant planets. Note that the equation has been earlier studied for a density of 0.6 g/cm^3 and a temperature of 3000 K which are typical of conditions needed for the production of metallic hydrogen under terrestrial conditions. On the basis of those researches, some important thermodynamic characteristics for such giant planets of the solar system as Jupiter and Saturn have been specified. In particular, we proposed an algorithm for finding the helium concentration in the central regions of those planets.

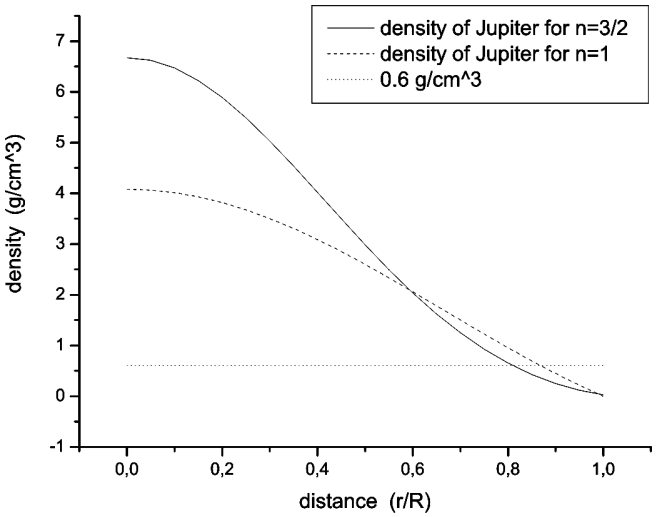

Fig. 1. Dependences of the Jupiter density on the distance from the planet center for various values of polytrope index

2. Equation of Mechanical Equilibrium of the Planet

The equation of mechanical equilibrium of the planet looks like [6–8]

$$\frac{1}{r^2}\frac{d}{dr}\left[\frac{r^2}{\rho(r)}\frac{dP(r)}{dr}\right] = -4\pi G\rho(r). \tag{2.1}$$

Here, $P(r)$ and $\rho(r)$ are the planet pressure and density, respectively, as the functions of the distance to the planet center, and G is the gravitational constant. This equation describes a planet with a spherically symmetric substance distribution and without taking its rotation into account. The relation between the pressure and the density is conventionally described by the polytrope equation

$$P(r) = c\rho^{1+1/n}(r), \tag{2.2}$$

which follows from the assumption on the convective mechanism of heat transfer between different planet layers. Here, c is an arbitrary constant, and n the polytrope index.

The planet specificity reveals itself through the boundary conditions at the center and on the surface of the planet:

$$\rho(R) = 0, \tag{2.3}$$

$$\rho(0) = \rho_0, \tag{2.4}$$

$$c(1+1/n)\lim_{r\to R}\rho^{1/n-1}(r)\,\frac{d\rho(r)}{dr} = -G\frac{M}{R^2}, \tag{2.5}$$

$$\frac{d\rho(0)}{dr} = 0. \tag{2.6}$$

Here, M is the mass of the planet, R its radius, and ρ_0 the planet substance density at the planet center. The mass and the radius of the planet are considered to be known quantities, and the density at the center is an additional parameter of the problem. Four boundary conditions allow one to obtain the partial solution of the equation and determine the constants ρ_0 and c.

Making use of the substitutions $u = \rho^{1/n}$, $y = u/u_0$, and $x = \lambda r$, the equilibrium equation can be transformed into a dimensionless form

$$\frac{1}{x^2}\frac{d}{dx}\left(x^2\frac{dy}{dx}\right) + y^n = 0, \tag{2.7}$$

which is the Emden equation. The parameter u_0 is defined by the relation $\rho(0) = u_0^n$. Now, both the density and the pressure of the planet can be expressed in terms of the solution $y(x)$ of the Emden equation and the dimensionless radius of the planet x_1, the latter being the solution of the equation $y(x_1) = 0$:

$$\rho(r) = -\frac{x_1 M}{4\pi R^3 y'(x_1)}y^n\left(\frac{x_1}{R}r\right), \tag{2.8}$$

$$P(r) = \frac{G\,M^2}{4\pi(1+n)R^4\left[y'(x_1)\right]^2}y^{1+n}\left(\frac{x_1}{R}r\right). \tag{2.9}$$

The only unknown parameter is the polytrope index n. In the case $n = 1$, the Emden equation is linear and has an analytical solution. The latter is adopted to correspond to a partially degenerate electron gas. This value of the polytrope index is the most popular today [3, 5]. In Figs. 1 and 2, it corresponds to a density of about 4 g/cm^3 at the Jupiter center and a pressure of about 40 Mbar. The horizontal line corresponds to the density, at which hydrogen was obtained in the metallic state under terrestrial conditions. The figures demonstrate that, if $n = 1$, the favorable conditions for hydrogen to transform into the metallic state arise already at a distance of 0.1 radius from the planet surface. If $n = 3/2$, these conditions are satisfied at a distance of 0.2 radius from the planet surface, and the density and the pressure in the planet center are close to 7 g/cm^3 and 60 Mbar, respectively.

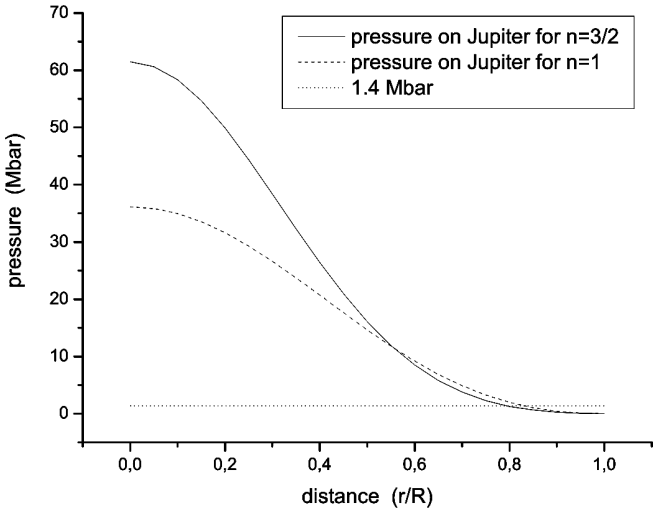

Fig. 2. Dependences of the Jupiter pressure on the distance from the planet center for various values of the polytrope index

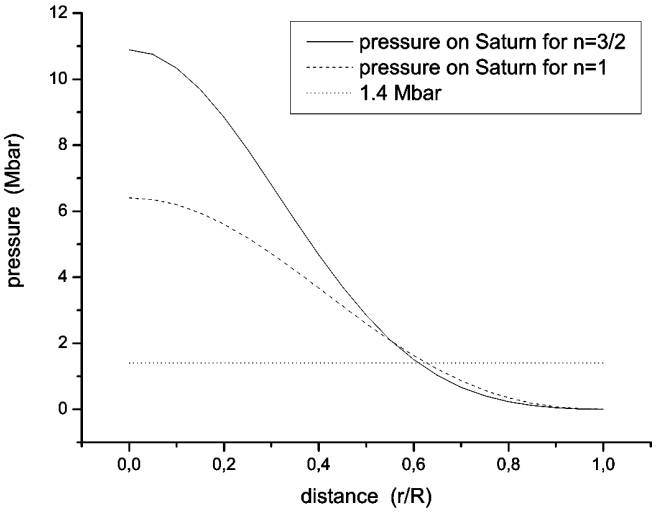

Fig. 3. Dependences of the Saturn pressure on the distance from the planet center for various values of the polytrope index

In this work, we adopt $n = 3/2$, which corresponds to a completely degenerate electron gas. As is shown in Fig. 3, the difference between the pressures in the central region of Saturn in the indicated cases of the polytrope index is rather substantial.

As is seen from Fig. 2, where the dependences for the pressure on Jupiter are depicted, the favorable conditions for hydrogen to transform into the metallic state also arise at a distance of 0.1 radius, at $n = 1$, and 0.2 radius, at $n = 3/2$, of the planet. Since two thermodynamic parameters simultaneously get necessary values at these points, the latter are to be considered as points that divide the metallic and molecular phases of hydrogen. The third thermodynamic parameter, the temperature, according to the equation of state that was studied in works [12–14], also has a necessary value of about 3000 K.

Since the temperature at the center of planets, according to various estimations, amounts to approximately 10000–20000 K, which is several percent of the Fermi energy, it is sufficient that the account of temperature effects to the internal planet energy be confined to corrections that are only linear in the temperature. Such a correction is the kinetic energy of the proton and helium subsystems. The temperature correction to the electron gas energy is quadratic in the temperature, so that it can be totally neglected, and the electron gas can be considered as completely degenerate. It is easy to show that, if $n = 3/2$, almost 80% of the Jupiter mass is located in the region of hydrogen metallization.

3. Model of Ideal Electron, Proton, and Atomic Gases

The polytrope index $n = 3/2$ corresponds to the models of classical and degenerate ideal gases. We apply the first model to describe the proton subsystem of metallic hydrogen and helium atoms. In so doing, we consider the planet substance to be chemically homogeneous and helium atoms to be neutral, which completely corresponds to the modern representation concerning conditions for helium metallization [15, 16]. We confine the consideration to the planet region, where helium metallization occurs.

Let c be the concentration of the electron gas. Let us define it as a ratio between the number of electrons and the number of protons and helium atoms. In this case, the pressure created by atoms and protons is

$$P_{p+\mathrm{He}}(\rho, T, r) = \frac{\rho(r)}{M_{\mathrm{H}}c + M_{\mathrm{He}}(1-c)} k_{\mathrm{B}} T(r), \tag{3.1}$$

where M_{H} and M_{He} are the masses of a proton and a helium atom, respectively; and $\rho(r)$ is the planet substance density which is determined from the equation of mechanical equilibrium for the planet. Correspondingly, for the density of electrons, we have

$$n_e(c, r) = c \frac{\rho(r)}{M_{\mathrm{H}}c + M_{\mathrm{He}}(1-c)}. \tag{3.2}$$

The second model – the model of degenerate ideal gas – is applied to describe the electron gas which is formed at the hydrogen metallization in the central region of the planet. The corresponding equation of state reads

$$P_e(\rho, r) = 2n_e(c, r)\varepsilon_F(c, r)/5, \tag{3.3}$$

where $P_e(n_e, r)$ is the pressure in the degenerate gas created by electrons at the distance r from the planet center, and m is the electron mass. Hence, if interactions are not taken into account, $n = 3/2$ for a mixture of hydrogen and helium, irrespective of whether they are in the molecular or metallic state. The total pressure that arises in the central region of the planet is

$$P(\rho, T, r) = P_{p+He}(\rho, T, r) + P_e(\rho, r). \tag{3.4}$$

The numerical analysis of this formula shows that both Jupiter and Saturn cannot consist of hydrogen only, because the pressure of electron gas is several times higher in this case than the pressure calculated from the equation of planet mechanical equilibrium, provided that the model of polytropic layer with $n = 3/2$ is used. If the electron concentration, as well as the concentration of hydrogen in the central region of the planet, amounts to only 0.761, those pressures are practically coincide for Jupiter. For Saturn, the limiting concentration of electron gas is 0.649. In our opinion, the main factor that is responsible for such a concentration is the availability of other elements – first of all, helium – in the planet structure. This conclusion has to be specified, first of all, by taking the proton subsystem into consideration, as well as interactions in the system.

Since the temperature-induced contributions to the thermodynamic potentials and the pressure are small corrections, the results of calculations of the planet temperature are sensitive to the electron gas concentration. At a concentration of 0.761, the temperature of Jupiter is zero. This means that it is the temperature positivity that fixes the upper limit of the electron gas concentration. At a concentration of 0.74, the temperature in the planet center achieves 20000 K. This circumstance explains the large divergence available in literary data concerning the temperature.

The planet temperature can be found by equating the pressures determined in the ideal gas and polytropic layer models. In this case, we obtain the temperature as a function of the distance to the planet center and the electron gas concentration. Nowadays, no additional information on the temperature can be obtained. To determine the planet temperature, another equation is needed, which would enable one to determine the electron gas concentration. As such, let us take the equation of state for interacting electron, proton, and helium gases. In this case, the role of interactions in the formation of pressure magnitude on the planet can be elucidated as well.

4. Internal and Free Energies

The Hamiltonian of the electron subsystem in metallic hydrogen can be taken in the form similar to that used for simple liquid metals [17]. The internal energy of the system is obtained by averaging the Hamiltonian over the Gibbs canonical ensemble

$$E = \langle \mathrm{H} \rangle = E_i + E_e + E_{ie}. \tag{4.1}$$

For the contribution of the proton subsystem to the energy, we have

$$E_i = \langle \mathrm{H}_i \rangle = N\frac{3}{2}k_{\mathrm{B}}T + N\frac{1}{2V}{\sum_{\mathbf{q}}}' V(q)[S^i(q) - 1]. \tag{4.2}$$

Here, T is the absolute temperature of the systems. The first term on the right-hand side is the kinetic energy of protons. The second one is the Madelung energy which makes allowance for the interaction between charged protons, nuclei, and ions. The neutral helium atoms give no contribution to this energy. The quantity $S^i(q)$ is the static structural factor of the proton subsystem.

The energy of the electron subsystem and the interaction energy of electron and proton subsystems are convenient to be examined together. Their sum – the ground state energy of the electron gas in the proton-induced field – can be expanded in a series in the electron-proton interaction:

$$E_e = \langle \mathrm{H}_e \rangle + \langle \mathrm{H}_{ie} \rangle = \sum_{n=0}^{\infty} E_n. \tag{4.3}$$

In turn, every electron-proton interaction term should be expanded into a series in the electron-electron interaction. For the zero-order term with respect to the electron-proton interaction, it looks like

$$E_0 = N\left(\frac{1.105}{r_s} - \frac{0.458}{r_s} - 0.058 + 0.016\,\ln r_s\right). \tag{4.4}$$

Here, r_s is the Brueckner parameter of nonideality. The first term corresponds to the kinetic energy of electrons, the second to the Hartree–Fock energy [18]. The third and fourth terms correspond to the correlation energy,

for which the Nozières–Pines interpolation formula [18, 19] was applied.

The term of the second order with respect to the electron-proton interaction – the so-called band structure energy – looks like [20–24]

$$E_2 = N\frac{-1}{4\pi^2}\int\limits_0^\infty \frac{\pi(q)}{\varepsilon(q)}V^2(q)S(q)q^2dq. \tag{4.5}$$

Here, $\pi(q)$ is the polarization function, and $\varepsilon(q)$ is the dielectric permittivity of the electron gas in the random phase approximation, which takes the exchange interaction and electron correlations into account in the local field approximation [25].

Helium atoms, providing their availability, give a contribution to the band structure energy. This contribution can be included by making the substitution

$$V^2(q)S(q) \to c(1-c)[V_{\rm H}(q) - V_{\rm He}(q)]^2 +$$

$$+c^2V_{\rm H}^2(q)S_{\rm H,H}(q) + c(1-c)V_{\rm H}(q)V_{\rm He}(q)S_{\rm H,He}(q) +$$

$$+(1-c)^2V_{\rm He}^2(q)S_{\rm He,He}(q), \tag{4.6}$$

where $V_{\rm H}(q)$ and $V_{\rm He}(q)$ are the formfactors for the electron-proton and electron-atom interactions, respectively; and $S_{\rm H,H}(q)$, $S_{\rm H,He}(q)$, and $S_{\rm He,He}(q)$ are the partial proton, proton-atom and atomic, respectively, pair structure factors [26, 27].

As was shown in works [13, 14], the third-order, with respect to the electron-proton interaction potential, term is essential only in the vicinity of the transition point of hydrogen into the metallic state. Its absolute and relative values quickly fall down with the growth of the density. Already at a density of the order of 1 g/cm^3, it amounts to a few percent of the second-order term. At densities of 5–7 g/cm^3 which are characteristic of the central regions of giant planets, it can be totally neglected. It is much more true for the third-order, with respect to the electron-atomic interaction potential, term, because it is much less than the electron-proton-interaction term of the third order at every density.

According to the definition of free energy

$$F = E - TS, \tag{4.7}$$

S is the entropy of the system. It can be taken in the hard-sphere approximation [26, 27],

$$S = S_{\rm gas} + S(\eta), \tag{4.8}$$

where

$$S_{\rm gas} = \frac{5}{2} + \frac{3}{2}\ln\left(\frac{M_{\rm H}^C M_{\rm He}^{1-C}k_{\rm B}T}{2\pi n^{2/3}}\right) -$$

$$-c\ln(c) - (1-c)\ln(1-c) \tag{4.9}$$

is the entropy of ideal proton and atomic gases, n is its density,

$$S(\eta)/k_{\rm B} = -2\ln(1-\eta) + 6\left(1 - \frac{1}{1-\eta}\right) +$$

$$+15c(1-c)\eta(1-\lambda)^{1.7} \tag{4.10}$$

is the interpolation formula for the contribution associated with the interaction between hard spheres, η is the total packing density for protons and atoms, and λ is the ratio between the diameters of proton- and atom-simulating hard spheres.

The only system parameter in the hard-sphere models is the packing densities for protons and atoms which are directly expressed in terms of corresponding hard sphere diameters. To find them, the idea of effective proton-proton pair interaction is used [28]. Its important property is that it contains no fitting parameters, but depends only on the system density. The hard sphere diameter, i.e. the minimal approach distance for protons at a given temperature, is determined from the condition of equality between the kinetic and potential energies of two protons at their approach to each other. The hard sphere diameter and the packing density for helium atoms are determined in much the same way [29].

5. Discussion of Results

In Fig. 4, the distributions of the pressure on Jupiter calculated in various approximations are depicted. The planet substance was assumed to consist of two components: hydrogen and helium. Hydrogen was assumed to completely dissociate into protons and electrons, and helium to remain in the non-ionized atomic state. This assumption is true only for the central region of the planet, provided that the distance to the center does no exceed 0.8 times the planet radius. The planet substance is considered as chemically homogeneous. The only unknown parameter of the system is the electron gas concentration. In the framework of the microscopic model, this parameter governs both the planet temperature and the pressure. For the further consideration, we

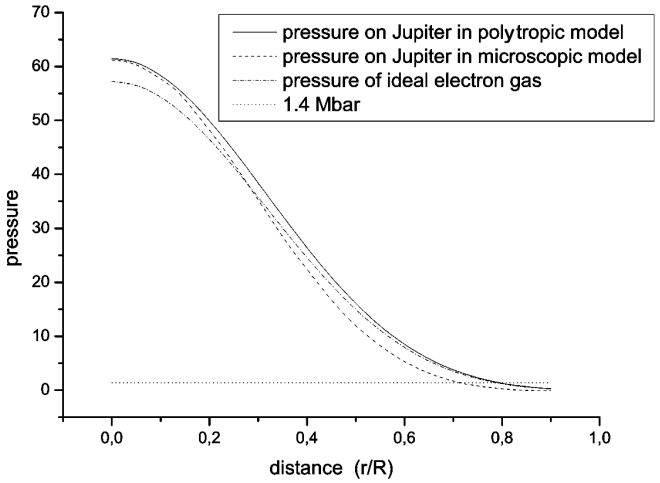

Fig. 4. Jupiter pressure calculated in the second order of perturbation theory with respect to the electron-proton and electron-atom interactions

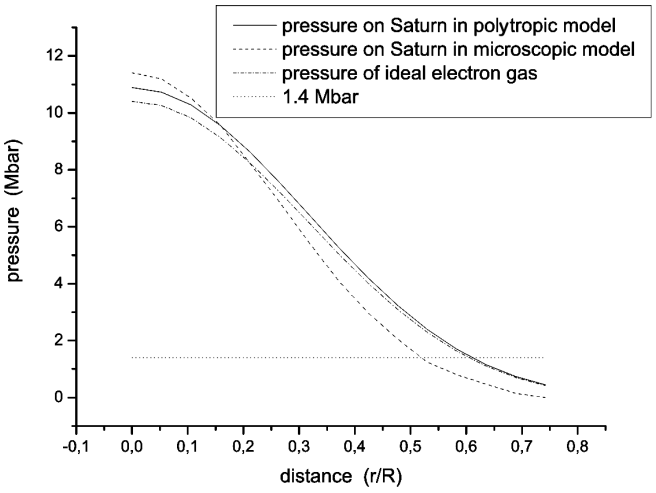

Fig. 5. Jupiter pressure calculated in the second order of perturbation theory with respect to the electron-proton and electron-atom interactions

select the value of this parameter that provides an equality between the pressures obtained in the framework of the polytropic model of the planet and calculated in the framework of microscopic model for a planet, which takes into account every interaction; both pressures are calculated at the planet center, where, owing to a high density of the electron gas, the role of interactions is the least. The corresponding electron concentration is equal to 0.747. In Fig. 5, the pressure distribution calculated using this value and the equation of state for the ideal degenerate electron gas is shown. It is evident that the model of ideal degenerate electron gas and the model of interacting electron-atom-proton liquid correspond rather well to the equation of state obtained in the framework of the polytropic model. At the same time, whereas the equation of state for the ideal degenerate electron gas better describes the pressure profile closer to the planet surface, the microscopic equation of state better describes the behavior of the equation of state, which was obtained in the framework of the polytropic model, closer to the planet center. In particular, the temperature at the Jupiter center, which corresponds to a concentration of 0.747, turns out to be 14000 K.

Note that the difference between pressures obtained in the framework of either microscopic or polytropic model of Jupiter testifies that the equation of state for an interacting system is not a simple power-law dependence. In the central region of Jupiter, where the electron gas density is extremely high, this difference is almost unnoticeable. When approaching the planet surface, the electron gas density quickly falls down, and this difference becomes substantial.

In Fig. 5, the solutions of the equation of state obtained in the framework of the polytropic, microscopic (taking interactions into account), and ideal-electron-gas models for Saturn are depicted. The electron gas concentration on the planet was taken to be 0.64. This concentration gives rise to a temperature of 4000 K at the planet center. For Saturn, the radius of the region, where the conditions are favorable for the hydrogen metallization, does not exceed 0.6 of the planet radius in the polytropic model and 0.5 of the planet radius in the microscopic model with interactions. Respectively, the mass of the planet substance that is concentrated in the metallization region amounts to 0.6 of the planet mass in the first case and to 0.5 of the planet mass in the second one. Hence, in the case of Saturn, the proposed microscopic model describes a considerably smaller region of the planet than that in the case of Jupiter. Accordingly, the accuracy of such a description is lower as well.

6. Conclusions

The model of almost free electrons is extremely good for the description of a substance under conditions that take place in the central regions of giant planets. The perturbation theory series of expansion in the electron-proton and electron-atomic interactions quickly converges. The contribution of interactions in a proton-helium system to the equation of state falls within the interval of 15–20%.

The concentration of conduction electrons for Jupiter amounts to 0.747, which testifies to the presence of many other substances (approximately 25%) – first of all, helium – in the Jupiter structure. The helium fraction in the central region of the planet is much higher than 18%, which is typical of the Jupiter atmosphere. The polytropic model is well substantiated for Jupiter.

The concentration of conduction electrons for Saturn amounts to 0.64, which testifies to the presence of plenty of other substances (about 35%) in the planet structure. The helium fraction in the central part of the planet has to be much higher than 11%, this value being typical of the Saturn atmosphere. The lower concentration of helium in the Saturn atmosphere than that in the Jupiter one gives rise to a lower concentration of helium in the central part of the planet. Hence, it cannot exceed 25%, the value characteristic of Jupiter. Therefore, the fraction of other substances in the Saturn structure is rather substantial. This circumstance makes the hydrogen-helium model used in this work rather approximative for Saturn.

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РІВНЯННЯ СТАНУ МЕТАЛЕВОГО ВОДНЮ ТА АТОМАРНОГО ГЕЛІЮ І ВНУТРІШНЯ БУДОВА ЮПІТЕРА ТА САТУРНА

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Р е з ю м е

Запропоновано рівняння стану суміші металевого водню та атомарного гелію. Досліджений інтервал тисків, температур і густин відповідає умовам найбільших планет сонячної системи – Юпітера і Сатурна. Вважається, що речовина планети являє собою суміш протонів, атомів гелію та електронів. Для знаходження тиску суміші використовується теорія збурень за електрон-протонною та електрон-атомною взаємодіями. Електронна підсистема розглядається у наближенні випадкових фаз. Взаємодії протонів, атомів, атомів і протонів враховуються у наближенні твердих сфер. Проаналізовано застосовність моделі політропного шару до моделювання внутрішньої будови Юпітера і Сатурна та запропоновано конкретне значення індексу політропи. Знайдено густину, тиск і температуру на Юпітері та Сатурні як функції відстані до їх центра. Оцінено можливі долі водню і гелію у складі планет.