

Mathematical Simulation of Complex Natural Systems

Yu. I. Sidorov

*Vernadsky Institute of Geochemistry and Analytical Chemistry, Russian Academy of Sciences,
ul. Kosygina 19, Moscow, 119991 Russia
e-mail: sidorov@geokhi.ru*

Received May 12, 2005

Abstract—The paper presents a review of publications devoted to the mathematical simulations of natural systems whose large spatiotemporal scales make impossible their adequate experimental modeling in nature. The studies include the modeling of the mineralogy of the surface rocks of Venus and Mars, fractional condensation from the gaseous constituent of the preplanetary nebula, the genesis of chondrites and the material of the Earth's upper mantle, and the evaporation of interstellar dust and the stratification of material in cooling planets.

DOI: 10.1134/S0016702906010095

INTRODUCTION

The complexity of natural systems (which consist of several components and phases) and the multifactor character of processes that occur in them, as well as the large spatiotemporal scales of these systems do not allow their adequate experimental modeling. This also fully applies to the outermost shales of other planetary bodies. Although the active studies of planets by spacecrafts have provided extensive material on the physics and chemistry of their atmospheres, surface topography, and the chemistry of the Venusian and Martian soils, the *in situ* analysis of the rocks composing the surfaces of these planets and the delivery of samples of these rocks remain complicated technical (and economic) problems.

This situation leaves practically no possibilities of studying these natural processes other than their computer simulations.

A theoretical apparatus for the solution of such problems is provided by chemical thermodynamics, which proceeds from the presumption that chemical equilibrium was reached and makes it possible to evaluate the phase composition and possible evolutionary pathways of the systems by comparing the free energy of their initial and final states without examining all intermediate stages, whose characteristics are often unknown. This was made possible thanks to long-standing systematic experimental studies that provided sufficient information on the physical, including thermodynamic, parameters of many natural substances.

PREDICTION OF THE MINERALOGY OF VENUSIAN AND MARTIAN SURFACE ROCKS

Geochemistry no. 12, 1978, published a paper [1] that presented an attempt to predict the mineralogical composition of Venusian surface rocks. In fact, this was

one of the first publications in the Soviet Union devoted to the numerical simulation of a complicated (13 components) multisystem of a planetary atmosphere and surface rocks. There is no doubt that the pioneer of these studies was Karpov [2], but his book was published by a regional publishing house and was hard to get for an interested reader.

This raises the reasonable question as to why such modeling had never been conducted previously, as the fundamentals of linear programming were published already in the 1950s [3]. Nevertheless, the main calculation algorithm for a complicated multisystem was developed only a decade later [4], and the first publication appeared in the Soviet Union only in the early 1970s. It is also pertinent to recall the equipment available for a researcher at that time, first of all, the availability of computers. Our simulations were conducted by M.V. Borisov, who used a computer program developed by Yu.V. Shvarov [5] at the Data Processing Center of the Moscow State University.

In practice, the problems were solved using data on the near-surface zone of the atmosphere from [6], the average compositions of seven types of terrestrial rocks, and consistent thermodynamic characteristics of 75 minerals, which were obtained by the analysis of literature data.

The main results of the estimations of the mineralogical compositions were as follows [1, 7]:

(1) the mafic and intermediate rocks may contain up to 40 vol % epidote; i.e., they are altered analogues of basalts and andesites;

(2) carbonates (dolomite) are stable only in the mineral assemblages of peralkaline rocks, and other, most probably chemically bound carbon-bearing species are absent from crustal rocks, or the contents of these species in the rocks are negligibly low.

It should be mentioned that the standard enthalpies of epidote, glaucophane, and other rock-forming phases (about 30 minerals) had been quantified and needed experimental verification, which was accomplished later [8, 9].

In late 1978, the *Venera 11* and *12* and *Pioner-Venus* planetary probes delivered precise instrumental data on the composition of the atmosphere and the P - T parameters at the surface of Venus [10, 11]. Inasmuch as the multisystem of the atmosphere and surface rocks is sensitive to the composition of the gas phase, the compositions of the altered basalts and granites should have been calculated by a new variant [12]. The principal conclusions of these calculations were formulated as follows: (1) the "soil" produced from the basalts may contain up to 20 vol % pyrite and anhydrite (~11 wt % S), and the alteration products of the granites contain ~1.9 wt % S; (2) minerals containing the OH group are unstable and are not formed even when the rocks interact with an atmospheric gas containing 0.135 wt % H_2O , i.e., a water concentration two orders of magnitude higher than that deduced from theoretical evaluations; (3) Fe is contained in the rocks in the form of Fe_2O_3 , i.e., hematite, while magnetite is unstable; (4) secondary mineral assemblages can undergo stepwise transformations even at relatively insignificant variations in the temperature and pressure (for example, a temperature decrease of ~40 K and a pressure decrease of ~25 bar, which corresponds to an altitude of +5 km, makes anorthite $CaAl_2Si_2O_8$ and clinoenstatite $MgSiO_3$ unstable in the basalts); and (5) interaction between the gases of the atmosphere with a matrix corresponding to the compositions of terrestrial acid rocks does not result in any significant mineral transformations; OH-bearing minerals are unstable; high-Al minerals, such as cordierite, can be formed; and, similarly to basalts, S is chemically accommodated in pyrite and anhydrite.

The likely most interesting conclusion presented in [12] is that the sulfur concentration in the peculiar Venusian regolith is much higher than in the Earth's crust. This conclusion was confirmed after the flight of the *Vega-2* spacecraft, whose landing module conducted the XRF analysis of the surface material of this planet and detected up to 5 wt % SO_3 [13], i.e., one order of magnitude higher than the concentration of this component in terrestrial sedimentary rocks.

The poorness of modern knowledge about the composition of the near-surface Venusian atmosphere and about the composition of the surface rocks (not to mention their petrology and mineralogy) makes ambiguous the interpretations of the physicochemical simulations of interactions between the surface material of the planet and chemically active gases. Nevertheless, such simulations provide the possibility of tracing the trends in the transformations of this material and of calculating the limits for the "binding" of chemically active volatiles in the altered analogues of igneous rocks.

We simulated the transformations of the surface material under the effect of chemically active atmospheric gases and the chemical weathering of some rock-forming minerals in the late 1970s for Martian rocks. Due to various reasons, the results of these simulations were not published in English [14, 15] and until two decades after their publication in Russian [16], and, thus, it seems to make sense to summarize here the main conclusions drawn from these simulations.

The calculated presence of talc, hematite, Ca and Mg sulfates and chlorides in the Martian soil and the absence of any significant amounts of carbonates from these rocks are consistent with the modeled composition of the Martian soil (modeled compositions of a mixture whose XRF spectra are the closest to those measured at the landing sites of the *Viking* module [17]). This provided sound reasons to suggest that the actual soil contains some amounts of crystalline phases that had reached equilibrium with the modern atmosphere, whereas the rest of the soil consists of metastable (including amorphous) phases. It seems quite probable that the occurrence modes of volatile components in the actual soil are similar to those predicted theoretically. Molecular water and the OH group are contained in montmorillonite, talc, and salts; sulfur is incorporated in Ca and Mg sulfates, and Cl is accommodated in Ca, Mg, and Na chlorides. The calculated contents of bound water in structural hydroxyl in the modeled Martian soil (2.2–2.5 wt % H_2O) are in good agreement with the estimates based on the sounding data and analyses accomplished by the *Viking* landers. This consistency suggests that a state close to chemical equilibrium was reached by the soil-atmosphere system (if ice is ignored) in terms of water steam. The calculations indicate that the amounts of water bound in the regolith may be higher if the water vapor concentration in the planet's atmosphere is higher.

PROBABILISTIC CHARACTER OF THE SIMULATIONS OF CHEMICAL EQUILIBRIUM

A new stage in the simulations of complicated systems at the stochastic modeling of natural processes was closely related to the designing of a system of thermodynamic information [18], whose usage was started only in the early 1990s, when the first database of thermodynamic constants of minerals and gases was compiled and when personal computers became available more widely.

The first study at this qualitatively new level was our research on the probabilistic character of thermodynamic equilibrium simulations, which was illustrated by the example of condensation in the preplanetary nebula [19].

The system consisted of approximately 250 individual compounds, and the calculations were conducted

for the points of a temperature succession within the range of 1800–300 K, with 50–200 individual calculations carried out at each point depending on the statistical stability of the calculated probabilistic characteristics [19]. It was demonstrated that, in the stochastic modeling of the condensation process of solid phases from a gas of solar composition, the probability of the appearance of some phases, such as Fe, corundum, gehlenite, perovskite, diopside, forsterite, enstatite, anorthite, microcline, and troilite is as high as 100% (these minerals compose group I). Group II includes nepheline, tremolite, Na-phlogopite, eastonite, fayalite, and ilmenite, whose probabilities are lower than 100% but higher than 50%. The probability of the formation of other condensates (which were combined into group III) is <50%, and this group comprises akermanite, wuestite, magnetite, sphene, rutile, Ti_3O_5 , ulvite, hercynite, cordierite, pyrope, pyrrhotite, FeO, spinel, andradite, almandine, and grossular (<20%).

The temperature range of condensation and the achievement of 100% probability of the appearance of group-I phases (except diopside and, to a lesser extent, microcline) is a few tens of degrees. This is caused by the relatively low uncertainties (<1%) in the free Gibbs energy of these phases. However, the most significant factor that affected the statistical trajectories for group I is the fact that these phases condense in the absence of “competition” with other condensates.

The latter fact is crucial for the configuration of the statistical trajectories for the group-II and group-III condensates and for diopside (group I), which competes with gehlenite and akermanite. This competition is particularly evident for Ti-bearing phases and for the replacements of diopside by tremolite, metallic iron by troilite, and alkaline feldspars and nepheline by micas.

The introduction of the concept of the existence probability of condensing phases made it possible to identify the appearance succession of these phases in the modeled systems, and the application of the expectation concept allowed us to accurately compare the results of calculations conducted by different techniques.

FRACTIONAL CONDENSATION FROM THE GASEOUS CONSTITUENT OF THE PREPLANETARY NEBULA

Our paper [19] was followed by a series of publications devoted to the modeling of fractional condensation from the gaseous constituent of the preplanetary nebula (PPN) and the subsequent transformation of the condensates into chondritic material.

The chronologically first publication dealt with the fractional condensation of a solid phase from a PPN gas compositionally identical to the photosphere of the sun [20]. In this paper, we examined the dynamic dependence of the reaction volume in which solid particles are formed on each of the previous condensation acts

with a correction of the bulk chemical composition according to the condensation mechanism, i.e., assuming the partial removal of chemical elements (that have condensed earlier) from the gas. We explored the dependence of the temperature of this volume on time and, consequently, derived a model for temporarily nonisothermal fractional condensation. A fundamental distinctive feature of our model was the possibility (provided by the dynamic dependence of the reaction volume on the previous history of the process) of the accurate incorporation of the “cooling time” parameter for the condensation space.

The condensation model was designed according to the following scheme:

(1) Isobaric–isothermal equilibrium was calculated for the initial temperature T and pressure P . If the equilibrium association contained no newly formed solid condensate, the temperature was reduced by ΔT_n , and the calculations were resumed.

(2) If the equilibrium system became heterogeneous (contained more than one phase), the mass of the chemical elements that produced the solid condensate was subtracted from the bulk elementary composition; the temperature was lowered by ΔT_{n+1} and the calculations were resumed.

(3) If a certain element was fully contained in the solid phase at the current temperature, the further calculations of the system were carried out without this element.

It should be mentioned that the functional dependence of ΔT_n is of exponential character and is controlled by the modeled rate of the temperature decrease: $\Delta T_n \cong 80\text{--}50$ K within the range of 1700–1500 K, and $\Delta T_n \cong 5$ K within the range of $T < 1400$ K.

Hence, at current P – T parameters, the chemical system was determined by the original solar bulk composition, except the masses of chemical compounds that have completely condensed during the cooling of the system to a given current temperature.

The equilibrium was calculated by minimizing the Gibbs free energy for a system with 18 independent components, including more than 100 gases and ~250 potentially present solid phases.

The modeling yielded a radially layered particle a few micrometers in diameter. The particle consisted of a corundum core, a silicate shell of melilites and pyroxene; the thickest near-surface iron–silicate zone (its origin is clearly pronounced in the trajectory of the growth dynamics of the particle in the form of three characteristic steps), and a surface film of Na and K sulfides. The zonal structure of the high-temperature condensate was reproduced experimentally [21].

It is worth mentioning the problem of the genesis of carbonates at the surface of condensing particles. As was demonstrated by thermodynamic calculations (Fig. 1), a temperature decrease (to below 550 K) should have been associated with the replacement of alkali sulfides

by the corresponding carbonates. A further temperature decrease should have resulted in the appearance of carbonates containing crystallization water, a fact that warrants including K and Na carbonates in the calculations in place of their sulfides.

Indirect evidence of the instability of “pure” Na and K sulfides in meteoritic material is provided by the only (at least, as far as our knowledge goes) find and description of a Na_2S inclusion in the metal phase of the unusual Kaidun meteorite [22].

Inasmuch as all major elements are condensed in the particle, its bulk chemical composition corresponds to the solar composition, except only for carbon and oxygen.

Of course, our study of fractional condensation was not pioneering, but it was the first to present a physical model for a condensed particle and its visual image (Fig. 2).

A model for the evolution of the condensation was published in [23]. It was underlain by the assumption that chemical processes at temperatures of 650–300 K can be ascribed to two weakly interacting reaction spaces: the volume of a solid condensate particle and the volume filled with the gas. Hence, with regard to the characteristic time of cooling for 1 K at low temperatures, which is most probably greater than 10^3 years [24], we assumed that the aforementioned temperature interval was marked by the spatial coagulation of single particles.

The origin of larger (millimeter-sized) conglomerate particles provides grounds to hypothesize that the surface layer through which the reaction volumes can interact was thick enough to almost completely block the diffusion of external gases into the particle but, at the same time, had an insignificant volume compared to the volume of this particle.

The mineral assemblage that was produced by fractional condensation and composed the particles was not in chemical equilibrium. The further evolution of the material making up the particle could occur within the volume constrained within the outer shell of the particle.

The approach based on the separation of the “fast” (gas) and “slow” (solid) volumes of the condensation reaction volumes and the assumption that chemical relaxation could be independent within each of these volumes was applied in [23] and, to the best of our knowledge, was the first effective attempt of modeling the non-equilibrium chemical dynamics of a cosmochemical object by methods of equilibrium thermodynamics.

“SOLAR CHONDRITE” MINERAL ASSEMBLAGE

The assumption that the lifetime of the particle (which presumably had an outer shell impermeable to external material) is long enough for the mineral assemblage of this particle to reach chemical relaxation

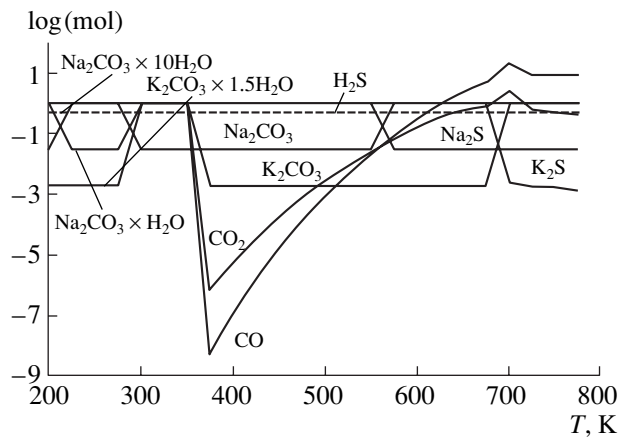


Fig. 1. Stability fields of Na and K sulfides and carbonates with the gas phase of PPN depleted after the condensation of major elements.

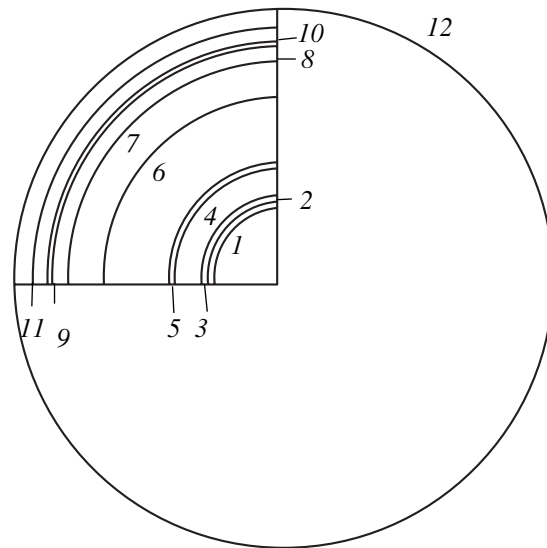


Fig. 2. Zonal structure of a condensate particle ($r \approx 2.25 \mu\text{m}$). (1) Corundum; (2) perovskite, corundum; (3) perovskite, gehlenite; (4) $\text{Ak}_{0.95}\text{Gel}_{0.05}$; (5) akermanite; (6) diopside; (7) forsterite, $\text{Di}_{0.25}\text{ClEn}_{0.75}$; (8) Fe, forsterite; (9) $\text{Ni}_{0.06}\text{Fe}_{0.94}$, forsterite; (10) (Ni,Fe), enstatite; (11) $\text{Ni}_{0.06}\text{Fe}_{0.94}$, enstatite, quartz; (12) Na_2S , K_2S .

provided the possibility of calculating the equilibrium composition by the method of isobaric–isothermal equilibrium. The assumption of the isobaric character of the process was based on the results of numerical simulations that have demonstrated that no degassing of the particle can occur within the temperature interval in question, and the isothermal character of this process was assumed based on the weak dependence of the chemical composition on temperature.

Table 1 lists the equilibrium composition of a particle obtained by nonequilibrated condensation from a gas of solar composition. These data clearly demonstrate that these were the first results obtained by simu-

Table 1. Modeled modal composition of the solar chondrite material

Mineral	vol %	Mineral	vol %
$Fo_{0.75}Fa_{0.25}$, olivine	58.8	$Ca_3(PO_4)_2$, whitlockite	1.0
$Di_{0.25}ClEn_{0.75}$, pyroxene	10.3	$FeCr_2O_4$, chromite	0.6
$Ab_{0.78}An_{0.16}Or_{0.06}$, feldspar	15.4	Mn_2SiO_4 , tephroite	0.5
$Fe_{0.94}Ni_{0.06}$	6.8	C, graphite	0.2
FeS, troilite	6.1	$FeTiO_3$, ilmenite	0.2

lating the mineral assemblage corresponding to the average composition of meteorites of the group of ordinary chondrites by the methods of equilibrium thermodynamics (without any assumptions concerning the extremal mechanisms of mass transfer). The mineral assemblage thus simulated was named “solar chondrite” (SC).

Table 2 presents the chemical composition of “solar chondrite” in comparison with those of H and L chondrites and with the condensate obtained by means of equilibrium condensation at $T = 600$ K. In our opinion, these data convincingly demonstrate that the chemical composition of “solar chondrite” corresponds to that of ordinary chondrites.

Table 2. Modeled chemical composition of the “solar chondrite” material in comparison with the compositions of H and L chondrites [25] and the composition obtained by equilibrium condensation at $T = 600$ K (“succession”)

“Solar chondrite”		H chondrites	L chondrites	“Succession”
component	wt %	wt %	wt %	wt %
SiO_2	33.5	36.41	39.70	35.77
MgO	24.0	23.09	24.58	25.76
Fe	13.0	17.45	7.3	17.81
FeO	13.0	8.87	14.33	–
FeS	7.8	5.67	6.06	19.24
Al_2O_3	2.4	2.60	2.81	0.25
CaO	1.9	1.87	1.92	0.21
Ni	1.6	1.68	1.07	0.18
Na_2O	1.0	0.93	0.94	0.09
Cr_2O_3	0.5	0.33	0.41	0.06
MnO	0.4	0.26	0.26	–
P_2O_5	0.4	0.18	0.22	0.10
TiO_2	0.1	0.11	0.11	0.13
K_2O	0.1	0.1	0.11	0.10

At $325 < T < 725$ K and $P = 10$ bar, the equilibrium composition of SC is invariant with respect to temperature, i.e., retains its phase homogeneity and the list of its mineral components. Below 325 K, alkaline plagioclase decomposes into microcline and albite, and the latter is, in turn, replaced by jadeite. This marks the end of the mineralogical transformations of the particle, and this assemblage remains unchanged to at least the temperature of H_2O condensation. At $T > 725$ K, free carbon is reversibly oxidized to CO and CO_2 . Until at least 1000 K, major elements (including K and Na) are retained in the solid phase at a practically unchanging mineralogical composition.

As is demonstrated by thermodynamic calculations, pressure does not affect the stability of the SC material within the range of 10^{-4} to 10 bar, the high-temperature stability limits lie above 650 and 1100 K, respectively, and the low-temperature limits are no higher than 200 K. Thus, at a pressure of $P = 10$ bar and temperatures of 200–1000 K, the major-element constituent of SC is solid and chemically stable.

LOW-TEMPERATURE EVOLUTION OF “SOLAR CHONDRITE” PARTICLES

The low-temperature evolution of SC particles was discussed in [26]. The major chemical components (other than H_2) of PPN remaining after gas condensation at $T = 250$ K are H_2O (~58 wt %), CH_4 (~26%), and H_2S (~3%). The long-lasting existence of SC particles (at $T < 250$ K) should result in the condensation of these gases (perhaps in the form of gas hydrates) at the surface of the particles. Since the task of [26] did not include the analysis of the condensation dynamics of these gases and the development of a model for low-temperature ($300 \text{ K} > T > T_{\text{cond}}$) nucleation, we proceeded from the assumption that H_2 does not condense at the surface of the particle, and H_2O , CH_4 , and H_2S condense at the surface of the particles in the form of gas hydrates and then diffuse in the condensate material. Vityazev *et al.* [27] explored the conditions under which compounds like $NH_3 \times 6H_2O$, $CH_4 \times 6H_2O$, and $N_2 \times 6H_2O$ are formed under P – T conditions corresponding to the cooling regions of PPN. The time of

Table 3. Modeled modal composition of the carbonaceous chondrite material

Mineral	vol %	Mineral	vol %
Mg ₆ (Si ₄ O ₁₀)(OH) ₈ , serpentine	44.2	(K,Na)-phlogopite	2.4
Fe ₃ O ₄ , magnetite	13.0	CaMg(CO ₃) ₂ , dolomite	1.8
Ca ₅ Mg ₅ Si ₈ O ₂₂ (OH) ₂ , tremolite	8.6	Na ₂ CO ₃	1.2
FeS, troilite	7.9	Ca ₁₀ P ₆ O ₂₄ (OH) ₂ , apatite	1.1
Na-montmorillonite	7.8	(Fe,Ni)Cr ₂ O ₄ , chromite	0.9
Mg ₃ (Si ₄ O ₁₀)(OH) ₂ , talc	7.1	MnCO ₃ , rhodochrosite	0.4
C, graphite	3.5	FeTiO ₃ , ilmenite	0.1

diffusion saturation is thereby much briefer than the lifetime of the chemical system in question.

Tables 3 and 4 present the calculated equilibrium mineral composition and the chemical composition, respectively, formed by the low-temperature condensation of H₂O, CH₄, and H₂S on a solar chondrite particle. The equilibrium composition corresponds to material like carbonaceous chondrite (point II in Fig. 3).

Our composition of carbonaceous chondrites is close to the composition of CM chondrites, whereas the material of the condensate obtained by means of equilibrium condensation is closely similar to CO chondrites (except the concentration of troilite). The latter fact is widely known. For example, Dodd [28] quotes the results of equilibrium condensation in the section devoted to carbonaceous chondrites.

In [26], we also considered the condensation dynamics that resulted in the material of enstatite chondrites. The following scheme of the condensation dynamics was simulated: (1) by a temperature of 1310 K, a particle was formed that had a composition in equilibrium with the residual gas (Table 5), with the composition of the particle corresponding to that of refractory inclusions in carbonaceous chondrites. During the expansion of the gas, particles of this composition could separate from the residual gas. One of the possible mechanisms of this separation was discussed in [29]. (2) Coagulation could begin to dominate over the condensate flux at a temperature of 1300 K. Table 6 demonstrates the mineral composition produced for this particle ($T = 675$ K, $P = 10^{-6}$ bar).

With regard for the condensation of S-, N-, and C-bearing components (FeS, MnS, FeC₃, Cr₂S₃, Fe₄N, and CrN), we calculated the equilibrium composition of the particle (Table 7), which corresponded to the material of enstatite chondrites (Fig. 3, point III). The chemical composition of the particle is shown in Table 8.

The model simulations of the heating of the “synthesized” material of enstatite chondrites (900 K) lead to the decomposition of carbonates and carbon reduction, a decrease in the forsterite content and an increase in that of enstatite (Table 9); i.e., the “synthesized” min-

eral composition approached the natural composition. The loss of osbornite and sinoite can be “counterbalanced” by the material in contact with the residual gas, in which NH₃ is one of the predominant compounds.

It should be mentioned that the application of techniques of equilibrium thermodynamics makes it possible to obtain only the limiting equilibrium (averaged) composition of the material of each of the chondrite types in question. The simulation of the whole chemical

Table 4. Modeled chemical composition of the carbonaceous chondrite material in comparison with the compositions of CM and CO chondrites [25] and the composition obtained by equilibrium condensation at $T = 300$ K (“succession”)

Carbonaceous chondrite		CM chondrites	CO chondrites	“Succession”
component	wt %	wt %	wt %	wt %
SiO ₂	28.4	27.57	33.58	33.60
MgO	20.3	19.18	23.74	24.19
FeO	16.9	20.28	24.20	17.84
FeS	11.0	8.66	6.05	22.44
Fe ₂ O ₃	7.0	–	–	–
H ₂ O	5.5	13.35	0.99	0.59
C	2.5	2.46	0.46	–
Al ₂ O ₃	2.1	2.15*	2.93*	0.24
CaO	1.6	1.66	2.64	0.20
NiO	1.6	1.53	–	0.16
Na ₂ O	0.8	0.63	0.58	0.09
Cr ₂ O ₃	0.5	0.36	0.49	0.07
P ₂ O ₅	0.3	0.30	0.32	0.10
MnO	0.3	0.21	0.20	0.27
TiO ₂	0.1	0.08	0.13	0.12
K ₂ O	0.1	0.05	0.14	0.09

* Data on other components are given for the Mighei (CM) and Lance (CO) meteorites.)

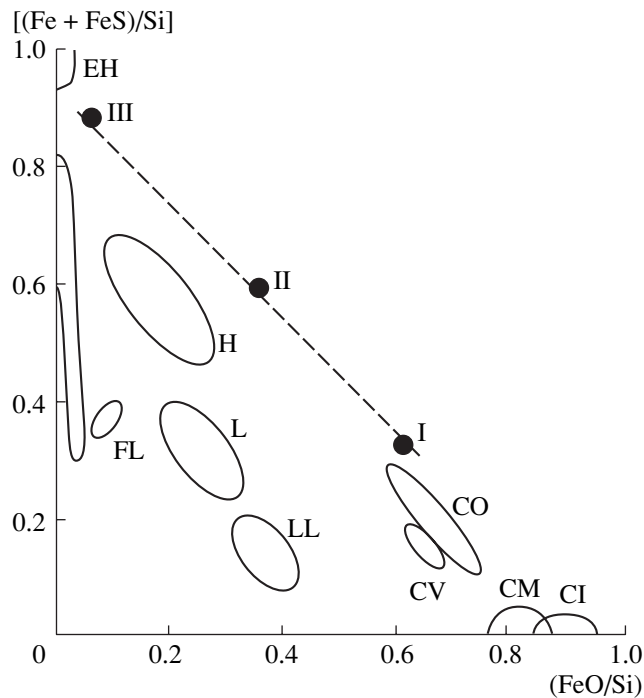


Fig. 3. Distribution of the modes of Fe occurrence in the modeled material of discrete chondrite types. (I) “Solar chondrite”; (II) carbonaceous chondrite; (III) enstatite chondrite.

and mineral diversity of naturally occurring meteorites would require the complete analysis of variants in the condensation–coagulation dynamics and the kinetics of the solid-phase reactions.

Our simulations [26] of the dynamics of fractional condensation and the subsequent interaction of the

“modeled” material with the residual (after condensation) gases of the preplanetary nebula during its cooling were the first to reproduce the probable mechanism that formed the material of all major types of chondrites. Our simulations with the use of equilibrium thermodynamics methods took into account nearly all accessory minerals found in meteorites.

PETROLOGICAL–GEOPHYSICAL MODEL OF THE EARTH’S UPPER MANTLE BASED ON “SOLAR CHONDRITE”

It was suggested in [23] that the equilibrium composition of the particle that was named “solar chondrite” corresponds to the average composition of terrestrial planets. This hypothesis was partially confirmed during the development of a petrological–geophysical model for the upper mantle of the Earth on the basis of SC [30] and the comparison of this model with the data of global seismology.

According to modern concepts, the primitive silicate mantle of the Earth consists of a hypothetical material named pyrolite [31]. Within the scope of the isochemical model for the Earth’s mantle of pyrolite composition, seismic discontinuities in it can be explained by phase transitions of Fe–Mg minerals, such as olivine → spinel at a depth of 400 km and the decomposition of spinel into the association of perovskite + magnesiowuestite at a depth of 650 km. The reasons for these stratifications remain largely obscure. We tried to return to Vinogradov’s [32–34] ideas about the chondritic model for the Earth’s material, which does not need any additional hypotheses to be invoked. Kuskov *et al.* [30] put forth the first consistent model of the composition and structure of the Earth’s upper man-

Table 5. Modeled modal composition of a particle of the high-temperature condensate

Mineral	vol %	Mineral	vol %
Ca ₂ Al(AlSiO ₇), gehlenite	81.6	CaTiO ₃ , perovskite	2.5
MgAl ₂ O ₄ , spinel	15.4	Al ₂ O ₃ , corundum	0.5

Table 6. Modeled unequilibrated modal composition of the enstatite chondrite material

Mineral	vol %	Mineral	vol %
Mg ₂ Si ₂ O ₆ , enstatite	68.2	Fe ₃ P, schreibersite	0.7
Fe _{0.94} Ni _{0.06}	14.7	MnS, alabandine	0.5
Mg ₂ SiO ₄ , forsterite	9.9	CaMg(Si ₂ O ₆), diopside	0.05
FeS, troilite	3.0	KAlSi ₃ O ₈ , microcline	0.01
Na ₂ S(cr.)	1.7	FeTiO ₃ , ilmenite	<0.01
FeCr ₂ S ₄ , daubreelite	1.3		

Table 7. Modeled equilibrium modal composition of the enstatite chondrite material

Mineral	vol %	Mineral	vol %
$Fs_{0.02}En_{0.98}$, pyroxene	69.0	MnS, alabandine	0.5
$Fe_{0.94}Ni_{0.06}$	14.9	MgS, niningerite	0.4
Mg_2SiO_4 , forsterite	8.9	CaS, oldhamite	0.02
FeS, troilite	2.6	Si_2N_2O , sinoite	<0.01
Na_2S (cr.)	1.7	$NaAlSi_3O_8$, albite	<0.001
$FeCr_2S_4$, daubreelite	1.3	TiN, osbornite	<0.001
Fe_3P , schreibersite	0.7		

tle on the basis of a cosmochemical model for the fractional condensation of the PPN material in the system Ca–Mg–Fe–Al–Si–Na–Ti–Ni–P–C–O–H–S and a petrological–geophysical model for the mantle material on the basis of a phase diagram for the fundamental petrological system CaO–FeO–MgO–Al–O–SiO (CFMAS). The consistence and closeness of this approach were considered proved if the mineral assemblages generated during the condensation of the PPN material were in agreement (if the cosmochemical and petrological–geophysical models of SC are valid) with available seismic data on the distribution of seismic-wave velocities and density.

As can be seen in the diagram of Fig. 3, the SC material lies on the line that passes through all other types of chondrites. This fact not only provides an additional argument for the most natural interpretation of the genesis of meteorites of different classes at different heliocentric distances, but also suggests the possibility that the terrestrial planets were produced from the SC material.

We have considered a new hypothesis of the origin of the Earth, a model for the differentiated solar-chondrite material. It was assumed that Fe–Ni alloy and FeS (the heavy components of SC) were the main differentiating phases of the Earth’s material. Because of this, the time span from the origin of the undifferentiated planet until the complete formation of its core was characterized by the evolution of the composition of this material from 10 vol % FeNi + 0.4 vol % FeS and corresponding contents of SiO_2 , MgO, and other components to the complete depletion of the mantle material in metallic Fe, Ni, and troilite and a corresponding increase in the contents of SiO_2 , MgO, and other components [30].

We limited ourselves to the development of a petrological–geophysical model of “solar chondrite” (PGMSC) that was based on the simulation of phase relations in the CFMAS system, which characterizes ~98–99 wt % the bulk composition of the Earth’s upper mantle. Table 10 presents the bulk composition of solar chondrite from which the compositions of the Fe–Ni alloy and accessory compounds were subtracted, and

the result was then recalculated into five major oxides. Our seismological models for the structure of the Earth’s mantle, with which the PGMSC was compared, were based on the basic PREM [39] and ACY-400 [40] models, which are consistent (as a first approximation) with the whole totality of seismic data on the Earth as a whole.

The calculations presented in [30] imply the conclusion that the SC model has physical characteristics that are in good agreement with all seismic data; the thermodynamic profiles of the SC material lie within the ranges of the seismic characteristics of both global seis-

Table 8. Modeled chemical composition of the enstatite chondrite in comparison with the average composition of enstatite chondrites [25]

Modeled composition		Average composition
Component	wt %	wt %
SiO_2	36.5	37.0
Fe	28.0	27.1
MgO	26.7	21.1
FeS	3.8	7.5
Ni	1.8	1.8
Fe_3P	1.3	2.0
Cr_2S_3	0.8	0.5
Na_2S	0.6	0.2
MnS	0.5	0.3
MgS	<0.1	0.1
C	<0.01	0.15
Al_2O_3	<0.01	1.45
CaS	<0.01	<0.1
K_2O	<0.01	0.1
Na_2O	<0.01	0.7
TiN	<0.01	–

Table 9. Modeled modal composition of the enstatite chondrite material

Mineral	vol %	Mineral	vol %
Mg ₂ Si ₂ O ₆ , enstatite	74.12	Fe ₃ P, schreibersite	0.7
Fe _{0.94} Ni _{0.06}	15.3	MnS, alabandine	0.5
Mg ₂ SiO ₄ , forsterite	4.5	C, graphite	0.2
MgS, niningerite	1.7	CaS, oldhamite	0.02
FeS, troilite	1.6	NaAlSi ₃ O ₈ , albite	0.01
FeCr ₂ S ₄ , daubreelite	1.3	TiC(cr.)	<0.001

Table 10. Comparison of the chemical compositions of the “solar chondrite” material and the Earth's mantle (calculated by different models and recalculated to the CFMAS system)

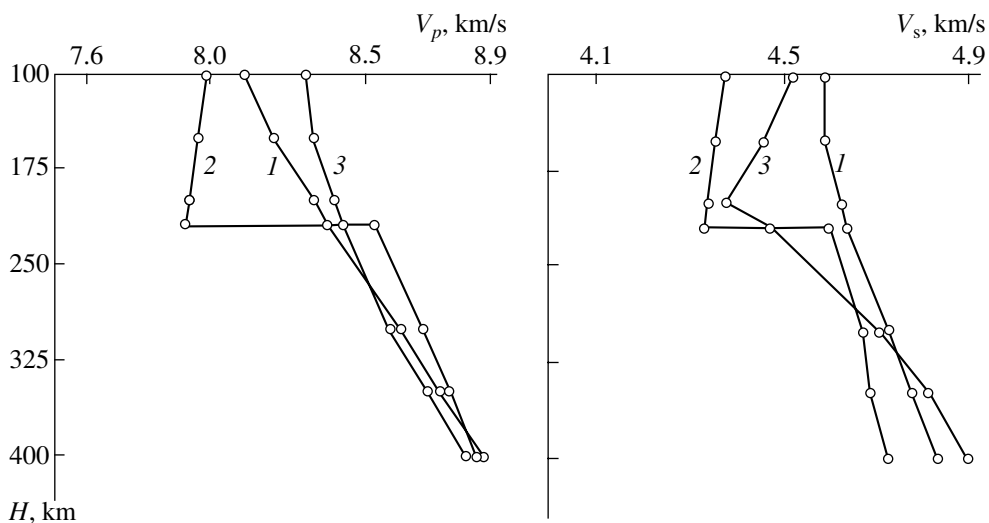
Component, wt %	SC	Ringwood, 1977 [35]		Morgan and Anders, 1980 [36]	Wanke, 1981 [37]	Saxena and Eriksson, 1986 [38]
		pyrolite	CI			
SiO ₂	48.3	45.9	49.1	48.8	45.4	42.7
MgO	34.7	38.7	34.7	34.7	38.3	39.3
FeO	10.7	9.0	9.4	9.3	8.7	9.9
Al ₂ O ₃	3.4	3.3	3.5	4.0	4.1	4.4
CaO	2.9	3.1	3.3	3.2	3.5	3.7

Note: Models: [36] seven components, [37] and [38] two components: (A) high-temperature and (B) low-temperature condensate.

mological models: PREM and ACY-400 (Fig. 4, Table 11).

Within the errors of the calculations and the accuracy of modern seismic data, the model of the upper mantle consisting of the “solar chondrite” material is compatible with the seismic constraints and does not

require any additional assumptions concerning the primary mantle material (such as pyrolite) or models in which the composition of the protomaterial is assumed to be a mixture of high- and low-temperature components (Table 10) and that do not suggest any physical mechanisms for the genesis of such mixtures.

**Fig. 4.** Seismic wave profiles for various models of the Earth's upper mantle: (1) PGMSC, (2) PREM, and (3) ACY-400.

MODEL FOR THE EVAPORATION
 OF THE INTERSTELLAR DUST MATERIAL

Our publication [41] was devoted to the evolution of an interstellar dust particle that moves in a gas of model chemical composition towards the hot central body, whose chemical composition is a parameter of the model. It was assumed that the radial velocity of the gas–dust system is of the order of the free fall velocity, but the velocity of a dust particle relative to the gas is low enough. Because of this, the material of the particle has enough time to reach chemical equilibrium with the ambient gas at any P – T point of the space through which the particle passes.

Since there is no direct reasons to postulate that the Sun's chemical composition is identical to the composition of the parent star of the protosolar nebula, the choice of the chemical composition of the dust particles was a separate problem. The inspection of models for the evaporation of material at temperatures below those of the complete evaporation of Fe-bearing components led us to conclude that the monotonous heating of the dust material should not have resulted in a decrease in the Fe/Si ratio. Because of this, the model composition of the interstellar dust material was chosen to be equal to that of a sample of extraterrestrial material that had the lowest Fe/Si ratio. We believed that such a sample could be the material composing the nucleus of Comet Halley [42]. We assumed that, up to the time when the drift of the particle began, the gas shell surrounding it consisted of hydrogen and helium and it became enriched in heavy ($m > 4$) components only in the process of particle evaporation.

It should be mentioned that this assumption could be reasonable enough if the drift of the particle was modeled for the early stages of the gravitational collapse that produced the proto-Sun and the protoplanetary disk. In fact, at least at high temperatures (>500 K), the particle is surrounded by an atmosphere that contains the material of particles that have evaporated previously. This led us to consider two marginal situations with the chemical composition of the gas that surrounded the particle during its drift. The model of “hydrogen flushing” (MHF) assumes that all evaporation products were blown out of the sphere of the thermodynamic influence of the particle by a hydrogen–helium flow. In the model of “stellar gas” (MSG), the particle evaporates in its own atmosphere, which was formed by the helium–hydrogen mixture and the products of earlier evaporation. It is reasonable to suggest that the actual gas that surrounded the particle during its drift had a composition intermediate between the two proposed above.

Figure 5 illustrates the evolution of the density of the non-evaporated material of a particle that drifts in P – T space during its equilibrium coexistence with the atmosphere modeled by the MHF and MSG conditions (lines 1 and 2, respectively).

Table 11. Earth's mantle density calculated by different models

H , km	P , kbar	T , K	ρ , g/cm ³		
			PGMSC	PREM [39]	ACY [40]
100	29.0	1103	3.382	3.373	3.368
		1203	3.367		
150	46.5	1343	3.400	3.367	3.363
		1393	3.393		
200	64.0	1473	3.432	3.362	3.350
		1543	3.422		
220	71.0	1543	3.441	3.36–4.366	3.388
		1603	3.433		
300	99.0	1623	3.503	3.484	3.505
		1673	3.497		
350	115.9	1673	3.538	3.513	3.547
		1723	3.532		
400	134.0	1723	3.574		
		1773	3.568	3.543	3.577
		1823	3.562		

Intermediate density values overlap the interval characteristic of the material composing planets and their satellites in the solar system. This corresponds to the density of condensate obtained in the model of the equilibrium condensation sequence [43] or to the density of the material obtained in the fractional condensation models [20].

The mineralogy of the material that was not evaporated suggests that its evolution provides record of the successive transformations of an assemblage with hydrated silicates into an assemblage rich in enstatite. The further drift of the particle makes possible the transition to an assemblage dominated by forsterite.

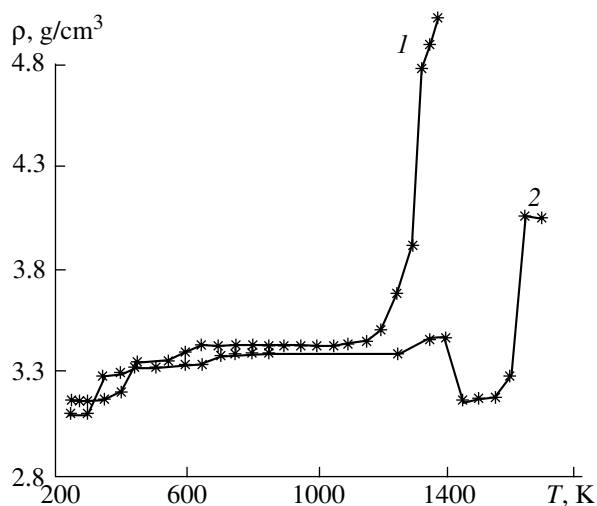


Fig. 5. Systematic variations in the density of an interstellar dust particle during its P – T drift in the gas medium. (1) Model of hydrogen flushing; (2) model of stellar gas.

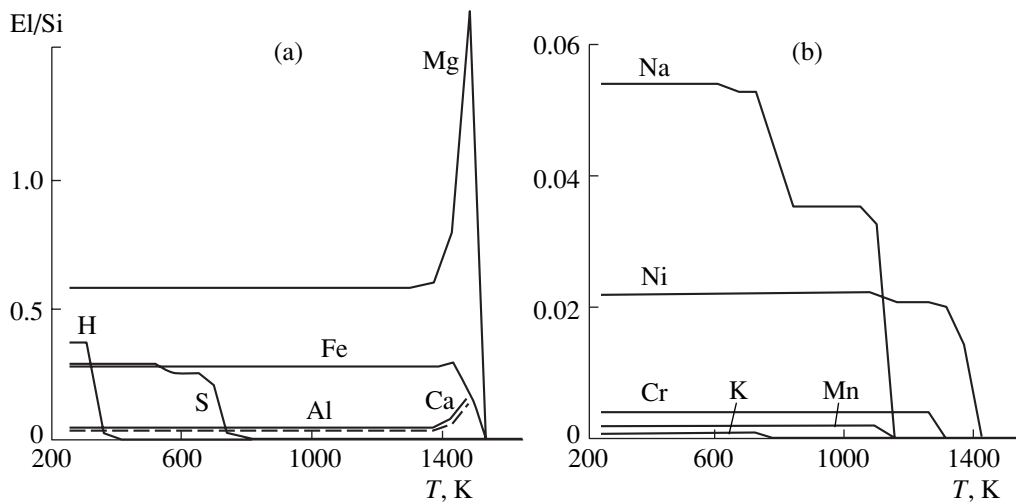


Fig. 6. Temperature dependence of the relative abundances (normalized to 1 Si atom) of (a) major and (b) trace elements.

The results of the modeling of the mineral composition into which all of the aforementioned associations are transformed, under the assumption of the equilibrium character of this composition, indicates that the major types of meteoritic material could be produced not only by the condensation of gas of solar composition [26] but also by the selective evaporation during the P - T drift of interstellar dust particles.

Figure 6 demonstrates the temperature dependences of the abundances of chemical elements (normalized to one atom of Si).

The results of our simulations of the selective evaporation of the interstellar dust material indicate that the density of the solid residue spans the interval of the

average density typical of the terrestrial planets, the moon, and the main types of stony meteorites [43, 44].

If the isotherm of 2000 K (the temperature of the complete evaporation of the dust component of PPN) passed between the orbits of Mercury and Venus, then the variations in the composition of the bodies of the solar system (except iron meteorites and Mercury) could be controlled by the selective evaporation of interstellar dust particles during their P - T drift.

It can also be hypothesized that, when the material composing the satellites of the giant planets was formed, interstellar dust variably lost its perfectly volatile components (contained in the ice) depending on the distance from the central body, but the origin of the Moon could be associated with the loss of not only ice, but also chemically bound volatiles and some major elements.

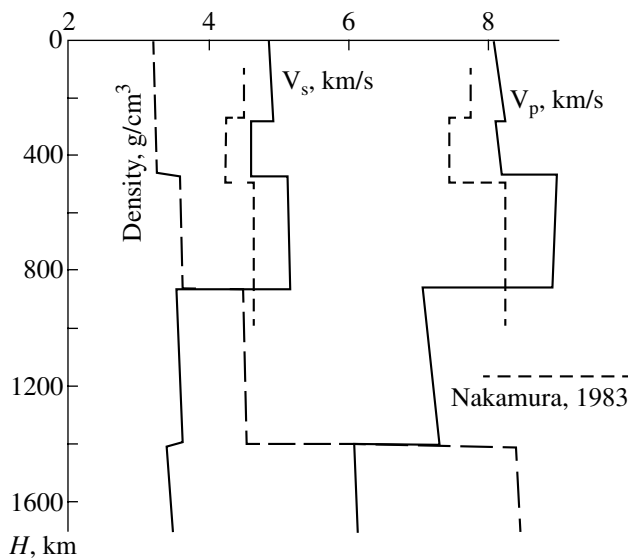


Fig. 7. Profiles of density and seismic wave velocities simulated for a body of lunar size and composition.

STRATIFICATION OF MATERIAL IN COOLING PLANETS

We also examined [45] a model for the equilibrium (finite) state of an isolated isothermal system whose mass and chemical composition make its gravitational and chemical potentials comparable. A physical prototype of such a system can be visualized as the terrestrial planets and the moon. For example, the gravitational potential at the surface of the Earth relative to an infinitely distant point is equal to -62 kJ/g, and the chemical potential of, for instance, quartz is ~ -29 kJ/g.

The modeling of the finite state of material was understood as searching for a distribution function of material within the planet. In our simulations, we took into account only the solid component of the planetary material because we believed that, at any given temperature that is obviously lower than the condensation temperature of major elements into mineral-forming compounds, the error related to the ignoring of the gaseous

(as well as liquid) phases of a system of mass comparable to that of planetary bodies should be much lower than the errors introduced by the uncertainties of the input thermodynamic data.

The possible existence of centrifugal, electric, magnetic, or other forces in the system was also disregarded, because we considered an immobile (not rotating) system that is electrically and magnetically neutral at any point.

The input data were the chemical potential, molar volume, mass, the adiabatic compression and shear moduli, and their derivatives for 35 “virtual” phases (quartz, forsterite, fayalite, and their high-pressure modifications, and others), as well as the mass and chemical composition of the respective planetary body.

The calculations yielded the radial distribution of the pressure and density, the composition of each layer, and seismic profiles for the Moon and Mars. Figure 7 shows the variations in the density and seismic wave velocities for a body of lunar size and composition. It can be seen that the profile of seismic waves practically coincides with the profiles obtained by direct seismic experiments on the Moon [46], and the shift of our calculated profiles for V_p and V_s is equivalent to the temperature difference between the modern lunar interiors and the temperature of 300 K at which the calculations were conducted.

Also we have analogously simulated (at a temperature of 300 K) a system of composition corresponding to the evaluated composition of Mars [47].

The modeling of the equilibrium state of isothermal self-gravitating systems that are catalyzed to the final evolutionary point (the prototypes of these systems are planetary bodies) allowed us to evaluate how distant from this state are bodies that have not yet finished their physicochemical evolution. This also provided us with insight into the evolution of the differentiation processes that currently take place in the interiors of the planets [48].

CONCLUSIONS

Our papers published over the past quarter of a century have demonstrated the possibility of solving equilibrium thermodynamics problems by numerical techniques in application to a variety of natural processes. We also attempted to follow, even if fragmentarily, the evolution of material from interstellar dust to its distribution in the shells of planets.

Model simulations of the interaction of the surface material of Venus with the planet's gaseous shell allowed us to evaluate the phase composition of the rocks and minerals in which perfectly volatile components are accommodated and enabled us to predict an elevated sulfur content in the Venusian surface material. Our evaluations were verified by the results of the instrumental analysis of the planet's soil accomplished by the *Venera 13* and *14* and *Vega 2* planetary probes.

The calculations of the chemical interaction of the Martian atmosphere with the surface rocks were the first thermodynamic simulations that made it possible to evaluate the composition of the Martian soil at the landing site of the *Viking* module and to identify the minerals in which volatile components are most probably contained.

The application of the method of stochastic modeling resulted in the obtaining of reliable and stable solutions, which were based on feedbacks between the models and the reliable and trustworthy information: primary experimental data, whose errors are in agreement with the errors of the modeling results.

The study of the fractional condensation from the gas constituent of the preplanetary nebula provided the first evaluations (made with regard for the mass balance) of the mineral assemblage of the “model” unequilibrated material whose equilibrium phase and chemical composition corresponded to the composition of ordinary chondrites.

Our model simulations of the fractional condensation dynamics and the interaction of the “model” material with the residual gases of PPN during its cooling enabled us to obtain a material whose chemical and modal compositions were close to those of enstatite and carbonaceous chondrites.

Proceeding from the “model” material (so-called “solar chondrite”), we arrived at the conclusion that, within the errors of the simulations and the accuracy of modern seismic data, the model for the upper mantle consisting of this material satisfies seismic constraints. There are good reasons to believe that the modern composition of the Earth's upper mantle corresponds to the composition of this material from which the differentiation products were subtracted (the differentiation products are Fe–Ni and FeS, which produced the core of the planet).

The results obtained by simulating the selective evaporation of the material of interstellar dust demonstrate that the major types of meteorites could be produced not only by the condensation of gas of solar composition but also by selective evaporation during the P - T drift of an interstellar dust particle. The density of the residue after this process overlaps the average density range for the material of the terrestrial planets, moon, and the major types of stony meteorites.

Although the simulations of thermodynamic equilibrium in a self-gravitating system were not pioneering and had been previously conducted to analyze the final states of objects of stellar mass, they were principally new in Earth sciences and enabled the transition from the analysis of “point” thermodynamic systems to those distributed in space and, thus, approached the development of mathematical geochemical models for natural systems.

Considered together, our studies and publications mark a new important stage in the mathematical simulation of complicated natural systems. These investiga-

tions provided insight into the transformations of material from the gaseous constituent of the preplanetary nebula and interstellar dust particles to the evolution of this material in developing planetary bodies and its distribution in them, as well as the transformations of the material during the interactions of the surface rocks of the planets with their gas shells.

REFERENCES

- I. L. Khodakovskiy, V. P. Volkov, Yu. I. Sidorov, and M. V. Borisov, "Mineralogical Composition, Hydration, and Oxidation of the Venusian Outer Shell: A Preliminary Prediction," *Geokhimiya*, No. 12, 1821–1835 (1978).
- I. K. Karpov, A. I. Kiselev, and F. A. Letnikov, *Chemical Thermodynamics in Geochemistry and Petrology* (Akad. Nauk SSSR, Irkutsk, 1971) [in Russian].
- G. B. Dantzig, *Programming in Linear Structures* (Comptroller. USAF, Washington, 1948).
- W. B. White, S. M. Johnson, and G. B. Dantzig, "Chemical Equilibrium in Complex Mixtures," *J. Chem. Phys.* **28**, 751–795 (1958).
- Yu. V. Shvarov, Extended Abstract of Candidate's Dissertation in Geology and Mineralogy (MGU, Moscow, 1982).
- K. P. Florenskii, V. P. Volkov, and O. V. Nikolaeva, "On a Geochemical Model of the Venusian Troposphere," *Geokhimiya*, No. 8, 1135–1150 (1976).
- I. L. Khodakovskiy, V. P. Volkov, Yu. I. Sidorov, and M. V. Borisov, "Venus: Preliminary Prediction of the Mineral Composition of Surface Rocks," *Icarus* **39** (3), 352–363 (1979).
- Yu. V. Semenov, Yu. I. Sidorov, I. L. Khodakovskiy, *et al.*, "Standard Entropy of Minerals," in *Proceedings of All-Union Conference on Mineralogy and Petrology* (Kiev, 1981), pp. 96–102 [in Russian].
- G. G. Likhoidov, Yu. I. Sidorov, V. M. Gurevich, *et al.*, "Thermodynamic Characteristics of Glaucophane $\text{Na}_2\text{Mg}_3\text{Al}_2\text{Si}_8\text{O}_{22}(\text{OH})_2$ and Some Petrological Implications," *Geokhimiya*, No. 7, 1002–1013 (1982).
- B. G. Gel'man, V. T. Zolotukhin, N. I. Lamonov, *et al.*, "Gas Chromatography of the Venusian Atmosphere by the *Venera-12* Spacecraft," *Kosm. Issl.* **17** (5), 708–713 (1979).
- U. von Zahn, S. Kumar, H. Niemann, and R. Prinn, "Composition of the Venus Atmosphere," in *Venus*, Ed. by D. M. Hunten, *et al.* (Univ. Arizona Press, Tucson, 1983), pp. 299–430.
- I. L. Khodakovskiy, V. P. Volkov, Yu. I. Sidorov, *et al.*, "The Geochemical Model of the Venusian Troposphere and Crust according to New Data," *Geokhimiya*, No. 12, 1747–1758 (1979).
- Yu. A. Surkov, L. P. Moskaleva, O. P. Shcheglov, *et al.*, "Determination of the Elemental Composition of Venusian Atmosphere by the *Vega-2* Spacecraft: Procedure, Equipment, and Results," *Astron. Vestn.*, No. 4, 275–288 (1985).
- Yu. I. Sidorov and M. Yu. Zolotov, "Weathering of Martian Surface Rocks," in *Advances in Physical Geochemistry: Chemistry and Physics of Terrestrial Planets* (Springer, New York, 1986), pp. 191–223.
- A. I. Shapkin and Yu. I. Sidorov, "Thermodynamic Models in Cosmochemistry and Planetology," *Geochem. Int.* **41** (Suppl. 1), S1–S144 (2003).
- Yu. I. Sidorov and M. Yu. Zolotov, *Martian Surface Rocks and Soil* (Nauka, Moscow, 1989) [in Russian].
- A. E. Baird, A. J. Castro, B. C. Clark, *et al.*, "Sampling Strategies and Ground Support for Inorganic Chemical Analyses of Mars Regolith," *J. Geophys. Res.* **82**, 4595–4624 (1977).
- A. I. Shapkin, Extended Abstract of Candidate's Dissertation in Technical Sciences (GEOKhI AN SSSR, Moscow, 1985).
- A. I. Shapkin and Yu. I. Sidorov, "Chemical Equilibrium and Substance Condensation in the Preplanetary Nebula: Probabilistic Calculation," *Geokhimiya*, No. 2, 272–285 (1994).
- A. I. Shapkin and Yu. I. Sidorov, "Condensation-Related Differentiation of Matter in the Preplanetary Nebula," *Geokhimiya*, No. 5, 627–641 (1994).
- O. I. Yakovlev, V. S. Fainberg, A. I. Shapkin, and G. I. Ranendik, "Melt Evaporation under Fast Heating Conditions," *Lunar Planet. Sci.* **XVII**, 924–925 (1985).
- A. V. Ivanov, G. J. MacPherson, M. E. Zolensky, *et al.*, "The Kaidun Meteorite: Composition and Origin of Inclusions in Metal of an Enstatite Chondrite Clast," *Meteorit. Planet. Sci.* **31**, 621–626 (1996).
- A. I. Shapkin and Yu. I. Sidorov, "'Solar Chondrite': A Product of the Post-condensation Transformation of Preplanetary Nebula Matter," *Geokhimiya*, No. 6, 771–770 (1994).
- D. N. C. Lin and J. Papaloizou, "On the Structure and Evaluation of the Primordial Solar Nebula," *Month. Not. R. Soc.* **191** (1), 37–48 (1980).
- H. B. Wiik, "The Chemical Composition of Some Stony Meteorites," *Geochim. Cosmochim. Acta* **9**, 279–289 (1956).
- A. I. Shapkin and Yu. I. Sidorov, "The Condensation of Solar Gas and the Formation of Preplanetary Nebula," *Geokhimiya*, No. 8/9, 1147–1160 (1994).
- A. V. Vityazev, Yu. F. Makagon, and G. V. Pechernikova, *The Origin of the Solar System: Kinetic and Thermodynamic Aspects* (Nauka, Moscow, 1994) [in Russian].
- R. T. Dodd, *Meteorites: A Petrologic-Chemical Synthesis* (Cambridge Univ. Press, New York, 1981; Mir, Moscow, 1986) [in Russian].
- A. N. Simonenko and B. Yu. Levin, "A Possible Mechanism of the Mass Transfer within the Protoplanetary Nebula," *Meteoritika*, No. 42, 23–27 (1983).
- O. L. Kuskov, Yu. I. Sidorov, and A. I. Shapkin, "A Composition Model of the Earth's Mantle Formed from the 'Solar Chondrite' Matter," *Geokhimiya*, No. 8/9, 1140–1146 (1994).
- A. E. Ringwood, *Origin of the Earth and Moon* (Springer, New York, 1979; Nedra, Moscow, 1982).
- A. P. Vinogradov, "The Atomic Distribution of Chemical Elements in the Sun and Stony Meteorites," *Geokhimiya*, No. 4, 292–295 (1962).
- A. P. Vinogradov, "Meteoritic Matter," *Geokhimiya*, No. 11, 1275–1312 (1965).

34. A. P. Vinogradov, "The Chemistry of Planets in the Solar System," in *Plenary Reports to the 11th Mendeleev Conference on General and Applied Chemistry* (Nauka, Alma-Ata, 1975), pp. 139–169 [in Russian].
35. A. E. Ringwood, *Composition and Origin of the Earth* Res. School Earth Sci. A.N.U., no. 1299 (1977).
36. J. W. Morgan and E. Anders, "Chemical Composition of Earth, Venus, and Mercury," *Proc. Natl. Acad. Sci. USA* **77**, 6973–6977 (1980).
37. H. Wanke, "Constitution of Terrestrial Planets," *Phil. Trans. R. Soc. London*, **303**, 287–302 (1981).
38. S. K. Saxena and G. Eriksson, "Chemistry of the Formation of the Terrestrial Planets," in *Chemistry and Physics of Terrestrial Planets* (Springer, New York, 1986), pp. 30–105.
39. A. Dziewonski and D. L. Anderson, "Preliminary References Earth Model," *Phys. Earth Planet. Int.* **25**, 297–356 (1981).
40. J.-P. Montagner and D. L. Anderson, "Constrained Reference Mantle Model," *Phys. Earth Planet. Int.* **58**, 205–227 (1989).
41. A. I. Shapkin and Yu. I. Sidorov, "Physicochemical Evolution of the Interstellar Dust Material in the Process of Heating," *Geokhimiya*, No. 5, 423–426 (1996) [*Geochem. Int.* **34** (5), 378–383 (1996)].
42. E. K. Jessberger, A. Christoforidis, and J. Kissel, "Aspects of the Major Element Composition of Halley's Dust," *Nature* **332**, 691–695 (1988).
43. A. I. Shapkin and Yu. I. Sidorov, "*P–T* Dependence of the Density of the Nebular Condensate," *Geokhimiya*, No. 12, 1196–1207 (1997) [*Geochem. Int.* **35** (12), 1060–1070 (1997)].
44. A. I. Shapkin and Yu. I. Sidorov, "Evolution of Mineral Composition of Interstellar Dust Particles," *Exp. Geosci.* **6** (2), 79–80 (1997).
45. A. I. Shapkin and Yu. I. Sidorov, "Stratification in Cooled Planets," *Geokhimiya*, No. 12, 1226–1240 (1998) [*Geochem. Int.* **36** (12), 1109–1122 (1998)].
46. Y. Nakamura, "Seismic Velocity Structure of the Lunar Mantle," *J. Geophys. Res.* **88**, 677–686 (1983).
47. Yu. I. Sidorov and A. I. Shapkin, "Internal Structure of Mars: A Gravitational–Thermodynamic Model," *Geochem. Int.* **38** (Suppl. 3), S375–S382 (2000).
48. A. I. Shapkin and Yu. I. Sidorov, *Thermodynamic Models in Cosmochemistry and Planetology* (Editorial URSS, Moscow, 2004) [in Russian].