The effect of temperature distribution in the lunar mantle on joint inversion of geochemical (bulk chemical composition), seismic and selenodetic (GRAIL and LLR) data

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Abstract. Using Bayes inversion approach and Markov chain Monte Carlo method (MCMC), we studied the effect of temperature distribution in the lunar mantle on the chemical composition (concentrations of main oxides Al₂O₃, FeO, MgO) and seismic velocities in the mantle. The temperature and concentrations of the main oxides were calculated with thermodynamic methods for phase relations and physical properties modeling in the system CaO-FeO-MgO-Al₂O₃-SiO₂ using the Gibbs free energy minimization method. A set of geophysical data was used for the inversion (selenodetic: mean radius (R), mass (M), normalized moment of inertia (Is / MR²), Love number k2 and seismic data – seismic travel times (TT). The Moon is assumed to be viscoelastic, spherically symmetric, and consists of nine layers with constant physical properties in each layer: megaregolith, crust, four mantle layers, low viscosity zone (LVZ), liquid outer core and solid inner core. Physical properties in each zone are assumed to be constant. The division of the mantle into layers was performed in accordance with the seismic model. The concentrations of the main oxides were set equal in the three upper layers of the mantle; the magma ocean model was used to calculate oxide concentrations in the lower mantle.

Two types of geochemical models of bulk composition of the Moon were considered: 1 - models with similar to silicate Earth Al₂O₃ content, 2 - models enriched in Al₂O₃ (> 4.5 wt.%). Linear temperature profiles in the mantle were considered, the temperature was set in the middle of the mantle layers at depths of 150, 375, 625 and 1000 km. At a depth of 150 km, the temperature was set at 600 °C; in the lower mantle, it varied from 1000 to 1400 °C. For both types of models and wide temperature range in the lower mantle, it is possible to obtain distributions of the main oxides concentrations in the mantle which are consistent with a given Al₂O₃ and FeO bulk composition. Calculated concentrations and velocities in the mantle are in good agreement with the results obtained by other authors.
1. Thermodynamic approach
The main goal of this study was to combine geophysical and geochemical information using a thermodynamic approach and calculate a consistent model for the composition and internal structure of the Moon. The inverse problem is solved using thermodynamic modeling approach of phase relations and physical properties in the five-component system CaO-FeO-MgO-Al₂O₃-SiO₂ with method of minimization of Gibbs free energy and a consistent database containing the equations of state of minerals and solid solutions. The phase diagrams for a given composition were calculated using the THERMOSEISM software package [1]

2. Geochemical models of the bulk composition of the Moon
Geochemical models of the bulk composition of the Moon in terms of FeO and Al₂O₃ concentrations are shown in fig. 1. Most of the models are quite similar in concentrations of FeO, but the content of refractory oxides (Al₂O₃, CaO) can be different.

All models in fig. 1 can be divided into two groups: 1 - models with similar to terrestrial aluminum oxide content, 2 - models with higher than the Earth’s aluminum content. Analysis of these composition models of the Moon showed the following ranges of possible concentrations of basic oxides for both types of models: for the first type: 3.5 ≤ Al₂O₃ ≤ 4.5 (Al₂O₃ = 4.05 ± 0.35 wt.%) And for the second type: 4.5 ≤ Al₂O₃ ≤ 7.7 (Al₂O₃ = 5.91 ± 0.39 wt.%). For both types of models 10 ≤ FeO ≤ 14 (FeO = 12.25 ± 1.33 wt.%).

Figure 1 Geophysical and geochemical models of the total composition of the Moon (crust + mantle) and silicate Earth.

3. Geophysical data
Geophysical data used for inversion [2] (table 1): selenodetic data — mean radius (R), mass (M), normalized moment of inertia (Is / MR²), Love number k² from [3].

Table 1 Selenodetic Data Used to Constrain Internal Structure Models of the Moon
| Parameter                          | Value                                   |
|------------------------------------|-----------------------------------------|
| Mean radius (R)                    | 1737.151 km                             |
| Mass (M)                           | (7.34630 ± 0.00088) × 10²² kg           |
| Normalized mean solid moment of inertia (Is) / MR² | 0.393112 ± 0.000012 |
| Degree 2 potential tidal Love number (k²) | 0.02422 ± 0.00022 |
| Monthly quality factor (Qm)        | 38 ± 4                                  |
| Annual quality factor (Qa)         | 41 ± 9                                  |
The Apollo mission data on travel times from [4] was used: a total of 318 (183 for P waves and 135 for S waves) from 59 sources (24 deep-focus events, 8 near-surface moonquakes, 19 meteoroid impacts, 8 artificial).

The error in determining the nth arrival time (\(\sigma_{\tau n}\)) is written as follows:

\[
\sigma_{\tau n} = \sqrt{\sigma_{n,r}^2 + \sigma_{n,e}^2}
\]

(1)

where \(\sigma_{n,r}\) and \(\sigma_{n,e}\) read time error and the event time error of nth travel time data, the error \(\sigma_\tau\) was taken from [4]. This makes possible to obtain solutions consistent with geochemical constraints.

4. The model of the Moon

We apply a viscoelastic spherically symmetric model of the Moon consisting of nine layers: mega-regolith, crust, four layers of the mantle, low viscosity zone (LVZ), liquid outer core and solid inner core. The mantle is divided into layers according to the model [5]: the first layer (Mantle 1) —34– 250 km, the second layer (Mantle 2) —250 - 500 km, the third layer (Mantle 3) -500 - 750 km, the fourth layer (Mantle 4) - 750 - ~ 1250 km (to the border with LVZ, which thickness is calculated from the inverse problem solution). In each zone, physical properties and concentrations are considered to be constant. When solving the inverse problem, conditions of non-decreasing density with a depth are imposed.

The crustal thickness is 34 km [6] (including a 1 km mega-regolith layer). The composition of the crust is taken according to [7]. Concentrations of \(\text{Al}_2\text{O}_3\) and \(\text{CaO}\) in the mantle are related by the chondritic ratio \(\text{CaO} / \text{Al}_2\text{O}_3 = 0.8\).

Concentrations of main oxides are considered to be equal in the three upper layers of the mantle (layers Mantle 1 - Mantle 3), and when calculating concentrations in the lower mantle (Mantle 4), the magma ocean hypothesis was used [8, 9], according to which the concentrations of the main oxides in the lower mantle are equal to the average concentration in the overlying layers (upper mantle + crust) and equal to the bulk concentration in the silicate Moon [10].

![Possible temperature profiles in the lunar mantle](image-url)
5. Inversion

In this work to calculate parameters of the internal structure of the Moon Bayesian inversion approach was used — an effective method for solving inverse nonlinear problems, such as modeling the internal structure of planetary bodies [11]. This study utilizes Markov chain Monte Carlo (MCMC) algorithm to infer the parameters of the lunar internal structure. The solutions of the parameters and their uncertainties were obtained from the posterior distribution which was sampled by the MCMC algorithm. Then, the likelihood function \( L(m) \), which is a measure of misfit between the model predictions and the observations is written as

\[
LHF = \exp\left(-\frac{(d_{\text{obs}} - d_{\text{cal}}(m))^2}{2\sigma_{\text{mass}}^2} - \frac{(d_{\text{obs}} - d_{\text{cal}}^{\text{MOI}}(m))^2}{2\sigma_{\text{MOI}}^2} - \frac{(d_{\text{obs}} - d_{\text{cal}}^{k2}(m))^2}{2\sigma_{k2}^2} - \frac{(d_{\text{obs}} - d_{\text{cal}}^{2q_a}(m))^2}{2\sigma_{2q_a}^2}\right)
\]

where \( d_{\text{obs}}, d_{\text{cal}}(m) \), \( \sigma, \sigma_n \) denote observed data, data calculated from the model \( m \), uncertainty of the observed data, and \( m \)th seismic travel time, respectively (similar to [2]). To combine geophysical and geochemical data, bulk concentrations of aluminum and iron oxides are included in the into LHF (\( A_{\text{bulk}} \) and \( F_{\text{bulk}} \)).

For the first type of models (\( A_{\text{bulk}} = (Al_{2}O_{3})_{\text{bulk}} = 4.05 \pm 0.35 \text{ wt.\%} \)), For the second type: \( A_{\text{bulk}} = (Al_{2}O_{3})_{\text{bulk}} = 5.91 \pm 0.39 \text{ wt.\%} \). \( F_{\text{bulk}} = (FeO)_{\text{bulk}} = 12.25 \pm 1.33 \text{ wt.\%} \) was assumed to be the same for both types of models.

Calculation of the composition and physical properties of the lunar mantle was carried out in the range of oxides, covering a set of potentially possible lunar compositions [7, 10, 12, 13 and others.] (wt.%): 25 \( \leq \) MgO \( \leq 45 \%), 40 \leq SiO_{2} \leq 55 \%, 5 \leq FeO \leq 15 \%, 0,1 \leq CaO, Al_{2}O_{3} \leq 7 \%.

6. Results

As a result of the inversion of geophysical and geochemical data for each temperature profile (Fig. 2), the concentrations of the main oxides in the mantle, the seismic velocities in each layer, the outer liquid and solid inner core sizes, and the seismic velocity and density in the LVZ were obtained (Fig. 3). The images in the figures show the results with a step on the temperature in the lower mantle of 100 °C.

The calculation results for the first type of models (with a bulk Al_{2}O_{3} content close to Earth) in Fig. 3 and are shown and in Fig. 4 for the second type of models (with a bulk Al_{2}O_{3} concentration higher than the values for the silicate Earth). The general trend of increase / decrease of each of the parameters is maintained up to a temperature of 1250 °C. With further increase in temperature, the solution ceases to follow the observed dependence.

When the temperature in the lower mantle is 1400 °C, an obvious separation of the solution occurs for all parameters for both types of models, and the value of the calculated parameters for these solutions are unrealistic due to geochemical and geophysical constraints. At a temperature of 1300 °C, for the first type of models, anomalous values of Vp velocity in the lower mantle were obtained. For second type of models at a temperature of 1300 °C for the concentration of Al_{2}O_{3}, the solution shows two peaks in histograms. It can be assumed that in the proposed formulation of the Moon model, the upper limit of the temperature in the lower mantle is 1250 °C.

Seismic velocities and density distributions for both types of models are in a good agreement with velocities according to the model [5] in the upper mantle (Mantle 1 and Mantle 2), Vp values obtained are higher in the Mantle 3, and in Mantle 4 it is lower than the most probable velocities in the model [5], however, they fit into the error bars of that model.

For all considered temperature profiles, at temperatures below 1400 °C, slight variations in the calculated concentrations of the main oxides in the mantle were estimated. The content of aluminum oxide (Fig. 3a) in the lower mantle (equal to its bulk concentration) is from 3 to 5 wt. % (the most likely value for all temperature profiles is about 4.1, which is close to the observed value of 4.05). In the upper mantle (Mantle 1 - Mantle 3), the Al_{2}O_{3} content for most models is from 2 to 4 wt.%, most likely from
2.5 for the lowest temperature profile to 3.5 for the high temperature profile. The concentration of FeO is 12.5–13.5 wt.% in the upper mantle, and almost the same in the lower mantle (12–13 wt.%, with the most probable value of 12.5) and is almost independent of the distribution temperatures (Fig. 3b). In the upper mantle, there is a slight decrease in the concentration of FeO with temperature increase. The MgO concentration (Fig. 3c) increases with increasing temperature and is 26-30 wt.% in the upper mantle and 24-30 wt.% in the lower mantle. In general, the obtained concentration values are consistent with the results obtained in [10, 11].

Figure 3 Probable distribution of calculated parameters in mantle 1-4 layers for type-1 models (bulk Al₂O₃ similar to Earth): (a) Al₂O₃ concentration; (b) FeO concentration; (c) MgO concentration; (d) seismic velocity Vp; (e) seismic velocity Vs; (f) density; (g) temperature.
Figure 4 Probable distribution of calculated parameters in mantle 1-4 layers for type-2 models (bulk Al₂O₃ higher than in the silicate Earth): (a) Al₂O₃ concentration; (b) FeO concentration; (c) MgO concentration; (d) seismic velocity Vp; (e) seismic velocity Vs; (f) density; (g) temperature.

P-wave seismic velocities gradually increase with increasing depth from 7.55-7.70 km/s in the upper mantle to 7.85-8 km/s in the lower mantle. There is a sharp increase of P-waves velocities in the upper mantle increase with an increase in temperature from 7.55-7.65 for the lowest-temperature model to 7.65-7.70 for a profile with a temperature in the lower mantle of 1250 °C. In Mantle 2, increasing of seismic velocities with increasing of temperature becomes less noticeable, in layer 3, the P-wave velocities are almost the same for all temperature profiles (7.70 -7.90 km/s with the most likely value of 7.81-7.82 km/s). In the lower mantle (Mantle 4), an inverse relation is observed between the velocity and temperature in the mantle — a decrease in velocity with increasing temperature from 8.0 to 7.85 km/s. Figures for S-waves also show an inverse dependence of velocities with temperature, however it occurs already at a shallow depth and is 4.4 - 4.5 km/s in Mantle 3, in Mantle 2 of S-wave velocities do not depend on temperature (4.42 - 4.44 km/s). In the upper mantle, the velocity slightly increases with increasing temperature from 4.41 to 4.43 km/s. S-waves velocities slightly increase with the transition from the upper layer of Mantle 1 to the layer of Mantle 2 and then decreases.
A similar temperature dependence (Fig. 3f) is observed for density, with the exception of Mantle 1, where the density decreases slightly with temperature increasing.

For the second group of models (with a concentration of Al₂O₃ higher than in the silicate Earth), the change in parameters with depth, as well as the effect of temperature distribution on parameters is similar to the first type, but the values themselves are somewhat different. The concentration of Al₂O₃ is 4.5 - 5 wt. % for the upper mantle and 5.5 - 6.5 wt. % for the lower mantle. The concentration of FeO is 12-13 wt. % in the upper mantle and 11.5 - 12.5 wt. % in the lower mantle.

Conclusions
1. The effect of temperature distributions in the lunar mantle on seismic velocities and concentrations of main oxides (Al₂O₃, FeO, MgO) in the mantle was studied for models with close to terrestrial bulk composition of Al₂O₃ and models enriched in aluminum oxide compared to Earth.
2. It was shown that for both types of models in a wide temperature range from 600 °C in the upper to 950 - 1250 °C in the lower mantle it is possible to obtain solutions that are consistent with geochemical and geophysical constraints. Calculated distributions of concentrations and seismic velocities are in a good agreement with the results obtained by other authors.
3. For a given mantle temperature distribution, the limiting temperature in the lower mantle is 1250°C.

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