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Development of technique of remote spectral sensing of technogenically loaded territories

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Introduction. The article considers the problem of monitoring technologically loaded landscapes. To solve it, the authors proposed an innovative method for studying the chemical composition of objects using direct spectral sensing means.

Problem Statement. The objective of this study is to consider the possibility of using spectral sensing to control the composition of soils in technogenically loaded territories.

Practical Part. To confirm the hypothesis that observing changes in the parameters of reflection spectra in non-selective areas will make it possible to establish the presence of basic biogenic macroelements for plants in the soil and evaluate its fertility, or determine the degree of contamination of the territory, a laboratory experiment was conducted using modern spectral equipment and multidimensional data calibration was performed.

Conclusion. The results of the analysis show the fundamental possibility of using spectral sensing in the monitoring of technogenically loaded territories using methods of multidimensional data analysis.

Keywords: monitoring, direct spectral sensing, soil chemistry, multivariate data analysis, state indices.

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Introduction. Over the past few years, man-made soil disturbances have reached unprecedented proportions as a result of the expansion of urbanized territories and the action of other anthropogenic factors. According to the State Report on the State and Environmental Protection of the Russian Federation for 2019, the area of disturbed land increased by 4.5 thousand hectares compared to 2018 and amounted to 1076.9 thousand hectares [1]. The report also notes the fact that over the past ten years there has been a tendency to increase the violation of land designated for industrial and other purposes (since 2010 there has been an increase of 119.9 thousand hectares). Thus, the organization of a monitoring system for territories near objects with a high technogenic load in order to control the quality of the environment and prevent possible degradation of the soil cover is an important and relevant topic at the moment.

The main problem of monitoring technogenically loaded territories today is to obtain objective and timely information about their condition.

There are field and laboratory methods of soil research [2]. Despite the fact that field methods are applied directly on the spot, they have a large measurement error, which does not allow us to correctly assess the quality of soils. That is why in most cases, the control of the state of the soil cover is carried out by a natural method with sampling and their examination in laboratory conditions. Laboratory research methods are quite accurate, but time-consuming. This method, as well as the field method, has a number of disadvantages, since for a real assessment of the soil cover of the territory, continuous recording of its state in real time is necessary. This is due to several things. Firstly, in areas with a high anthropogenic load, a sharp increase in toxicants in the soil cover is possible, the duration of generation of which may be much less than the interval between measurements. Secondly, laboratory studies require such work as taking a sample, transporting it to an accredited laboratory, directly analyzing and processing the data obtained, the output result may differ significantly from reality. And, thirdly, a reliable assessment of the total pollution flows is possible not by individual values of a number of observations, but by the integral of the controlled parameter over time.

The main advantage and feature of direct spectral sensing in comparison with the known methods is the study of the composition, structure and properties of objects at the research site without any preliminary operations [2]. Measurements can be carried out remotely by installing the equipment on any type of mobile platform or from the operator's hand. Spectral sensing is the basis for the creation of optical multi-sensor systems (MSS). MSS operate in a wide spectral range, which, when used, makes it possible to isolate specific spectra of soil reflection. This will allow optimizing the work on the removal of spectral characteristics and adjusting the monitoring process to the solution of specific tasks for the detection of a certain substance [3].

The idea of spectral sensing is that each chemical substance has its own spectral characteristics [3]. Observation of changes in the parameters of the soil reflection spectra will allow us to determine the presence of the main biogenic macronutrients for plants in the soil and assess its fertility. It is possible to determine the degree of contamination of the territory when detecting toxicants. The detection of individual substances by spectral sensing will also help to formulate the properties inherent to a particular soil under study, and to make a step-by-step description of the process of its self-purification after technogenic pollution.

Due to its significant advantages in comparison with other methods, the method of direct spectral sensing was chosen for monitoring and controlling technogenically loaded territories, the possibility of applying it in practice is considered in this article.

Problem Statement. The objective of this study is to consider the possibility of using remote spectral sensing to monitor the state of technogenically loaded territories.

The spectral characteristics depend on the composition of the soils. Since this technique is being developed for highly loaded technogenic landscapes, the analyzed samples taken for the experiment should correspond in their composition to the composition of the soils of such territories.

Initially, an assessment of the main elements that the soils of such landscapes can contain was carried out. Chemical indicators characterizing the properties of most soils were selected. Organic carbon was determined as a sign of soil humification, responsible for the presence of organic matter. Nitrogen in two types (nitrate and nitrite), sulfur and phosphorus were isolated as the main biogenic macronutrients necessary for the reproductive ability of plants. Potassium and sodium were taken into consideration as the main soil electrolytes. The ash content, which is responsible for the inert component of the soil cover, and humidity, which affects the spectral characteristics of soils, was also determined [4].

For the purposes of the research, the territories of agricultural lands located in the area of settlements of the Samara region were selected: Bolshaya Chernigovka, Kinel-Cherkasy, Rozhdestveno, Sergievsk and Khvorostyanka. Soil samples from the territories near the city of Togliatti that are not used for agricultural needs were also examined. At the sampling points of these samples, an increased content of phosphorus and nitrogen is observed due to man-made pollution. It is due to the close location of the existing enterprises (TolyattiAzot, KuibyshevAzot) and the currently liquidated plant Fosfor.

The initial data set on the chemical composition of the listed soils was created based on the results of quantitative and chemical analysis (QCA) of the laboratory of the Scientific and Analytical Center for Industrial Ecology of SamSTU.

Theoretical Part. A calibration database was created to build a regression model that can determine the content of chemical elements in the soil. The calibration data included the entire set of samples with previously clarified indicators, which will later allow determining the concentrations of real samples using the model.

An experimental setup was assembled to obtain the spectral characteristics of the samples. It included a portable computer with OceanView software, a USB cable for connecting a spectrometer, an incandescent light source, miniature OceanView STS-UV(UV) and STS-NIR (near-IR) spectrometers, a fiber-optic probe or collimator.

The installation used miniature spectrometers with different study ranges. The STS-UV spectrometer was used for taking reflection spectra in the ultraviolet radiation range (190-650 nm) and STS-NIR for near-infrared radiation (650-1100 nm). With this combination of spectrometers, it becomes possible to obtain spectra in the range from ultraviolet to near infrared, which completely cover the entire visible range. The equipment allows you to register a spectral signal, process it and display the results as a graphical representation on a computer monitor. These models of compact spectrometers are chosen as one of the most compact, and, therefore, suitable for installation on any type of mobile platform or for working in the field with the operator's hands device [5]. The use of two spectrometers made it possible to further conduct their comparative analysis and find out the range of the spectrum, where the response of the parameters under consideration is more clearly recorded.

A miniature spectrometer was connected to a fiber-optic probe. The probe technique is used for the convenience of taking readings at a remote distance from the spectrometer in the contact mode [6].

The advantage of such a technique is the use of a standardized lighting source without the influence of external sources. The probe has several main disadvantages: it increases the cost of installation, requires power for the lighting source, and requires close contact with the studied material. This makes it difficult to use it widely. Nevertheless, its use for research purposes is quite justified.

The system with a probe is replaced by a collimator for use in the field as a means of contactless or remote sensing. An optical collimator is a lens (in the simplest case, a concave mirror), in the focal plane of which is the matrix of the spectrometer. This arrangement makes it possible to obtain approximately parallel radiation beams. The spot from which the reflection spectrum is taken does not increase when the spectrometer moves away from the sample surface. In this case, a broadband incandescent lamp is used as a radiation source. It gives an almost uniform radiation power over the entire studied range. The radiation source was placed to the side of the sample location at a distance of about 10 cm, just like the spectrometer itself. The angle between the axes of the incident radiation and the collimator was 45 degrees, which simulates the position of the sun during field work.

The reflection spectra were recorded from each sample placed on a flat surface in an air-dry and wet (under a layer of water 1 mm thick) space. This made it possible to simulate the operation of the spectrometer at the time of precipitation. The spectral brightness of soils largely depends on their composition, which determines both the size of the particles composing the soil and the possible level of moisture content. An increase in soil moisture leads to a decrease in its reflectivity in the entire spectral range of reflected radiation [7].

The examples of the obtained spectra for different sites are shown in Fig. 1 and Fig. 2.

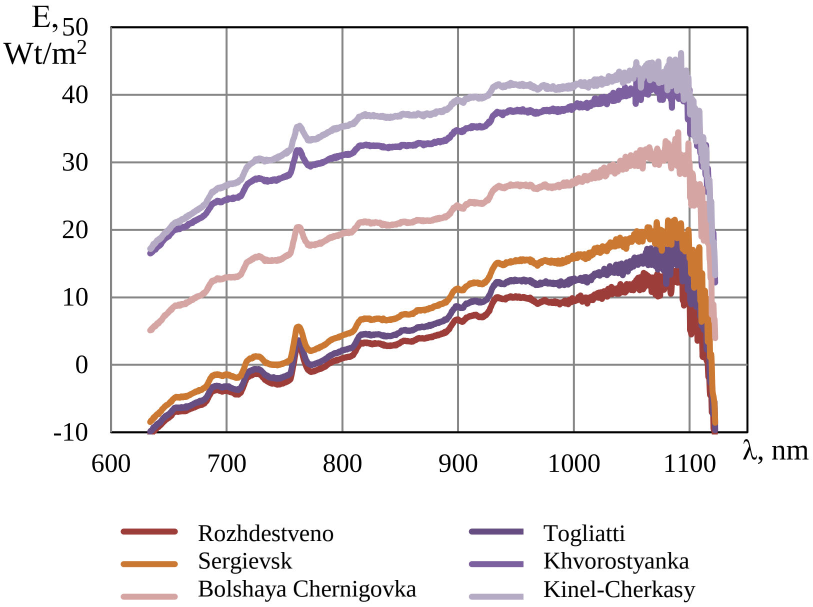

Fig. 1. Spectra of the studied samples from different sites, taken in the NIR range

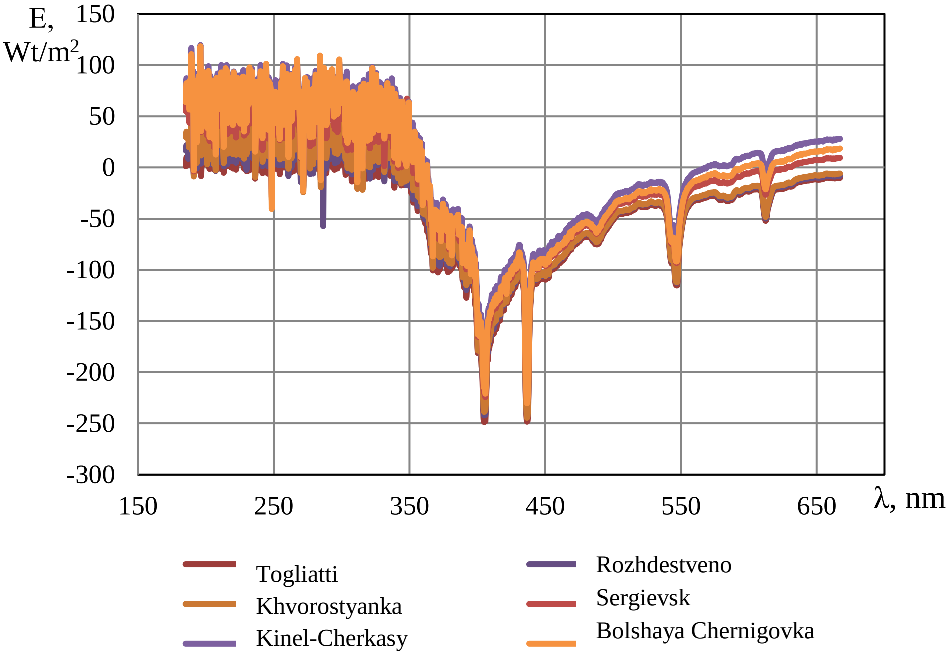

Fig. 2. Spectra of the studied samples from different sites, taken in the UV range

Since during the laboratory experiment it was possible to remove clear spectral curves, presumably characterizing the elemental composition of soil samples, and to obtain some generalized model of the state of the studied samples, the next stage of the work was to assess the possibility of using such a research method in practice in the field. Due to the fact that the laboratory analysis of soils took a long time, and the deterioration of weather conditions did not allow unhindered work in the field, it was decided to use the same soil samples for these works as in the preliminary laboratory experiment. The studied samples were placed on an testing site in the open air. To do this, the sample was rolled out on a site of about 0.25 square meters, and then the spectrum was taken in the same way as at the laboratory stage. At the same time, the reflection spectrum was influenced by weather conditions and the position of the sun.

Then the cross-validation procedure was performed [8]. That is, the spectra were cross-validated on full-scale soil samples under real conditions with 1/5 segmentation. As a training set, an array of data from laboratory studies of the spectral characteristics of soil samples was taken. A segment of 20% of the total number of samples was examined as unknown samples, and an assessment of the coincidence with the existing model was carried out.

Cross-validation refers to statistical methods that are used to evaluate the application of a model method in real conditions. Validation is usually used to compare theoretical data with practical data, because it is easy to understand, easy to implement, and leads to a reliable estimate, which usually has a lower bias than other methods. Its main advantage is working with the existing samples without the need for sampling.

The reflection spectra were recorded from every fifth sample of the studied soils, and a separate set of spectra was formed. Then the procedure was repeated with the second samples in each five. And so on for the formation of five independent sets.

When working on sites, there was no need to adjust for brightness, since the captured spectra were normalized. The integration time was also specially selected to ensure the optimal position of the spectral curves. In addition, software standardization was actually carried out, which significantly reduced the interfering influence of the environment.

As a result, the spectral characteristics of the samples were obtained, which were then compared with the previously obtained laboratory values.

In order to reduce the spread of the results of the spectra taken from the soils at the model sites, the cross-validation cycles were carried out with different partitions, and the obtained values were averaged.

When comparing the captured spectra in the laboratory and real conditions, a coincidence of the results was found. The average square deviation was no more than ten percent, which once again confirmed the similarity of the two experiments. This error is due to the normalization of the spectrum, so we can say that with the actual application of the method, it may be even smaller.

Comparison of dry and wet samples showed that the spectral curves obtained when shooting the spectrum of wet samples are smoother and well distinguishable from each other (Fig. 3). Thus, some peaks recorded from dry soils are aligned during waterlogging. It was also found that in the presence of water in the sample, the so-called noise in the wavelength range from 950 nm and above decreases, i.e. the definition area increases.

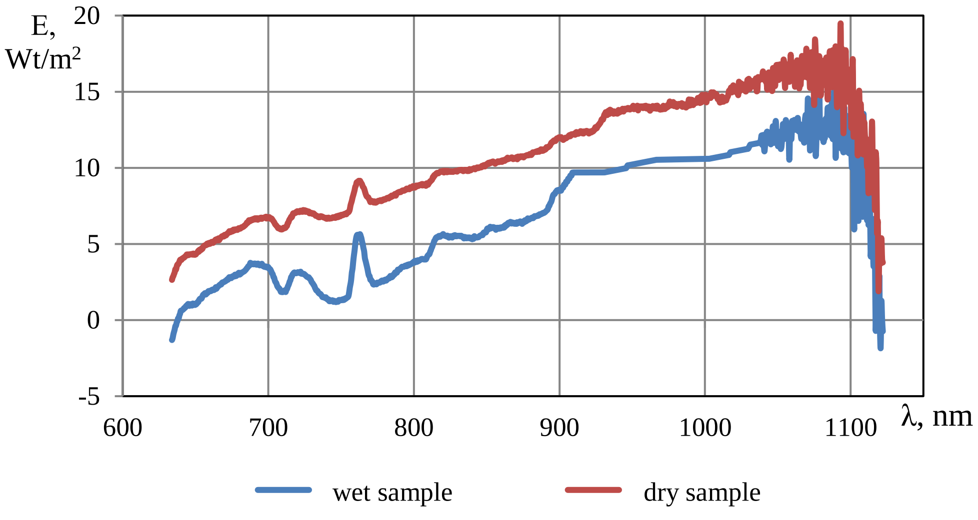

Fig. 3. Comparison of the spectra of dry and wet samples

However, there may be a discrepancy in the results of the analysis of dry and wet samples. There is a decrease in the values of the spectral characteristics of the soil when water is added to it. In addition, you can notice a change in the angle of inclination of the spectral curve.

To identify the dependence of the shape and position of the spectral line on the composition of the samples, a multidimensional calibration was performed using the multidimensional analysis software package The Unscrsmbler X. Prior to the start of calibrations, to assess the uniformity of the data structure, the modeling was initially carried out using the Principal Component Analysis (PCA) method — one of the main ways to reduce the dimensionality of the data, losing the least amount of information (noise), and to present the data in the form of projections [9]. It allows us to identify groups of samples with similar properties in a multidimensional space and determine the connectivity (correlation) of this distribution with certain properties.

It was determined that the samples from different sites have spectral differences that are not related to the indicators specified in the list of determined indicators, and form separate groups. Nevertheless, there are common features even for the sections that are scattered in the space of the main components. In particular, it is possible to conditionally identify areas with the predominant presence of samples from one of the sites, which indicates the fundamental possibility of identifying the site based on the spectral characteristics of the samples taken on it. However, this was not the purpose of this work, and no further consideration of this issue was carried out.

When comparing the formed areas and the quantitative chemical composition of the studied soils, a connection between them was found. As it can be seen in the graph of accounts, the spectral characteristics of the soils of different studied sites were divided into groups according to the content of the largest amount of a certain component (Fig. 4). In area No. 2, samples of soil cover with a higher concentration of sulfur were mainly combined, in area No. 3 — potassium and sodium, and in area No. 4 — nitrite and nitrate nitrogen. Area No. 5 is characterized by more moistened samples than others. The presence of phosphorus is recorded everywhere, but in greater quantities still in the samples that fell into area No. 1.

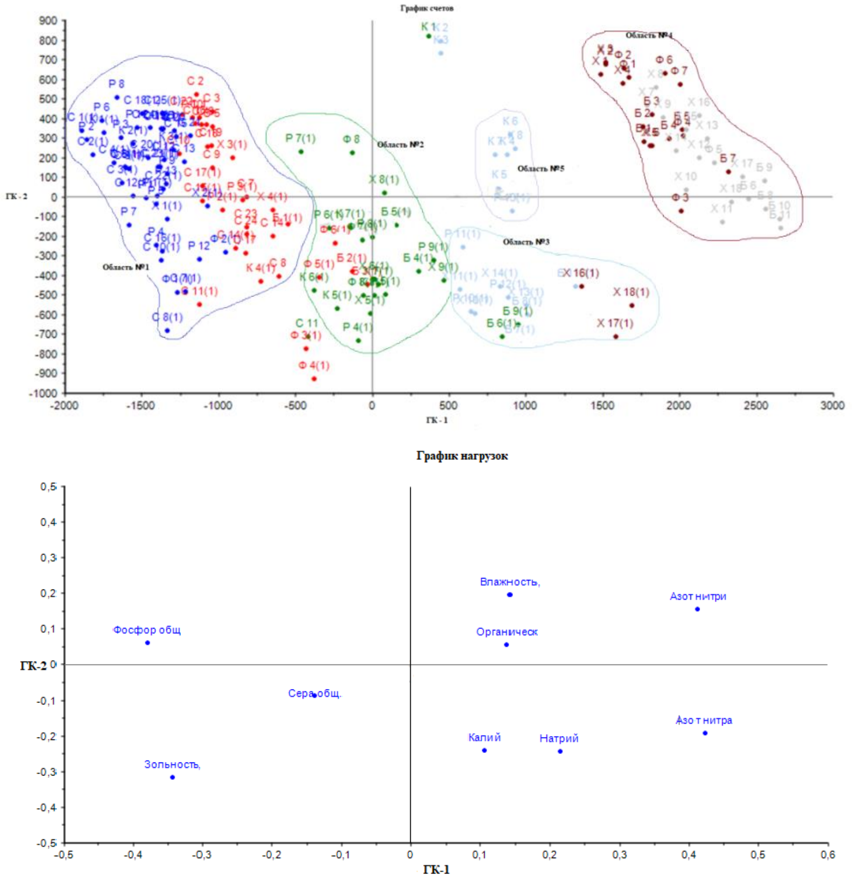

Fig. 4. Graph of samples (accounts) in a multidimensional spectral space:

ГК-1 — main component 1, ГК-2 — main component 2, С — spectral characteristics of the soils of the village of Sergievka, К — spectral characteristics of the soils of the village of Kinel-Cherkasy, Ч — spectral characteristics of the soils of the village of Bolshaya Chernigovka, Х — spectral characteristics of the soils of the village of KHvorostyanka, Р — spectral characteristics of the soils of the village of Rozhdestveno; Ф — spectral characteristics of Tolyatti soils

To identify structural features in the spectral data, a graph of variables (loads) was considered (Fig. 5). Despite the complementarity of the spectrometers in terms of the spectral range and spectral resolution of the features of the sensitive matrix, the UV and NIR-range spectra in multidimensional space are located in the form of disjoint groups of points, and modeling based on them should be carried out separately. There is a correlation of the chemical composition of soils with certain wavelengths.

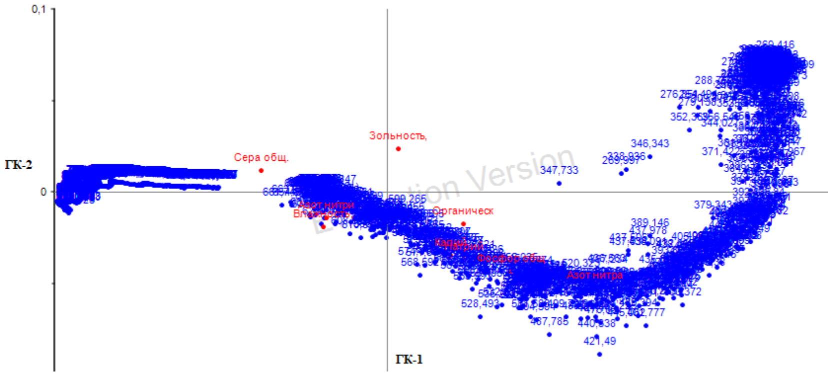

Fig. 5. Graph of loads of soil spectra of the UV range

To assess the data structure of the chemical composition and the possibility of separate determination in the array of information about the content of individual components, the modeling was also carried out in a multidimensional space using the principal component method (Fig. 6).

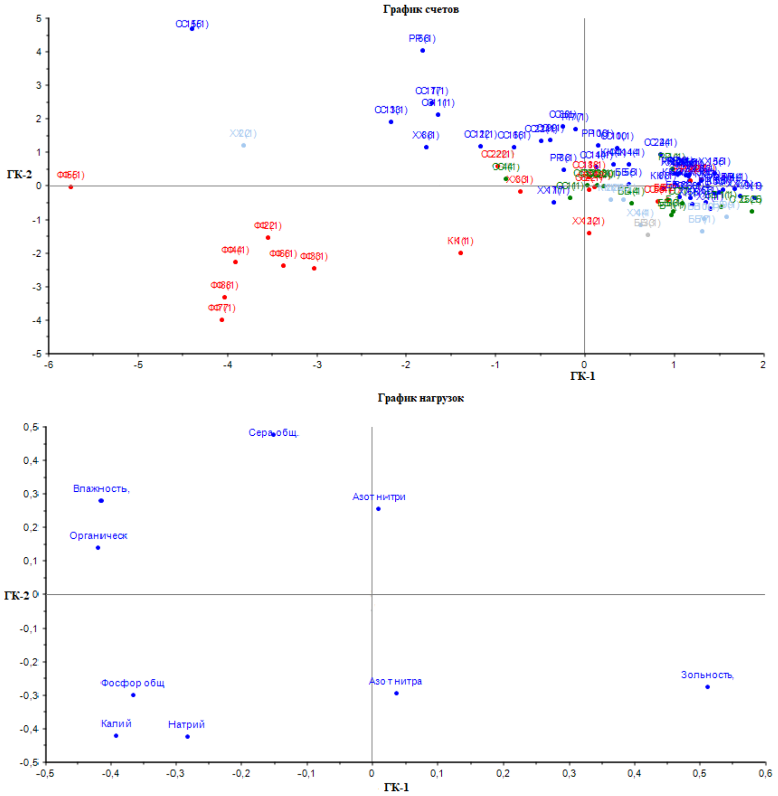

Fig. 6. Comparison of graphs of accounts and loads:

ГК-1 — main component 1, ГК-1 — the main component 2, С — spectral characteristics of the soils of the village of Sergievka, К — spectral characteristics of the soils of the village of Kinel-Cherkasy, Ч — spectral characteristics of the soils of the village of Bolshaya Chernigovka, Х — spectral characteristics of the soils of S. Khvorostyanka, Р — spectral characteristics of the soils of S. Rozhdestveno, Ф — spectral characteristics of Tolyatti soils

The obtained graphs allowed us to assess the situation for individual components and find a correlation between them. A correlation was found for nitrogen, phosphorus and sulfur, which can serve as a confirmation of the possibility of using spectral characteristics in assessing the quality of soil cover.

If we talk about samples from different sites, they were coordinated near the beginning of the axis of the chart of accounts, which may indicate their high dependence, i.e. similarity in the presence of a certain component, for example, nitrite nitrogen, which falls into a similar area on the load graph.

It can also be concluded that there is a negative correlation of nitrite and nitrate nitrogen in the samples. Nitrite nitrogen turns into nitrate nitrogen during the oxidation process, and this correlation is logical. The same conclusion can be drawn from the inverse correlation of such characteristics as humidity and ash content [10].

The graphs for estimating the prediction accuracy for all the chemical elements under consideration were analyzed (Fig. 7). The mean square deviation (R-Square) for phosphorus reaches 46 percent, which suggests that the model is already workable even under conditions of sufficiently high noise, fuzziness, as well as the influence of other factors and compounds. For such a non-contact method of determination, which will be used in the field, the obtained mean square deviation is acceptable for conducting a preliminary assessment of the content of a chemical element in the soil cover.

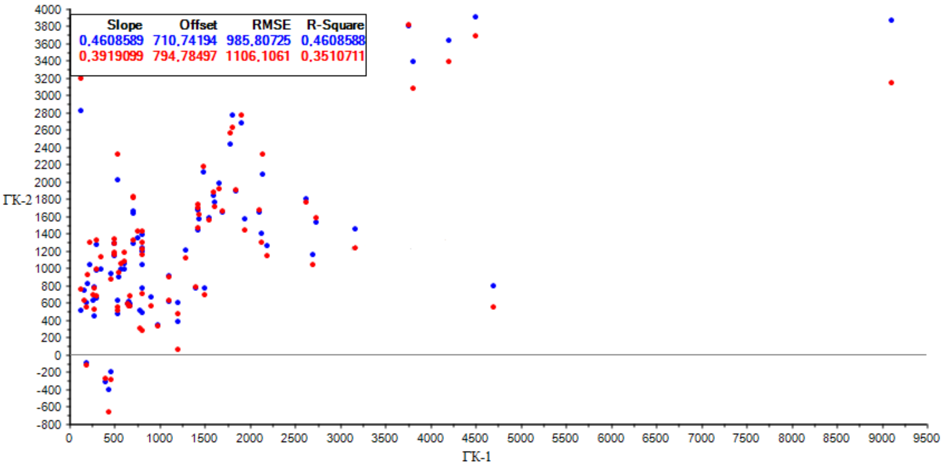

Fig. 7. Graph of estimation of prediction accuracy

In general, this model confirms the independence of the determination of soil components. The obtained result confirms the possibility of using spectral characteristics in assessing the quality of soils.

However, the use of full-spectrum models is often difficult, since it requires fast processing of significant data arrays and their long-term storage. There is a need to develop more convenient ways to work with multi-factor assessment systems for soil condition. To increase the information content, an indexing method is proposed in the format "more component content — less component content" [4].

Currently, there are about 160 variants of vegetation indices [11]. They are selected experimentally, based on the known features of the spectral reflectivity curves of vegetation and soils. The main advantage of indexes is their availability at different levels of probing with minimizing the mathematical processing of the received data. However, most of these indices are used to describe the state of vegetation cover, not soil. Thus, the use of indexing to assess the state of the soil cover is an important part of the description of the state of the objects of research and modeling.

The created calculated criteria, consisting of several intensities at certain wavelengths, may have a better correlation with the desired concentrations than directly with the spectra. They do not give absolute values, but in relative terms they can be well used in modeling the state of soils. At the same time, in the future, the use of these indices will provide an opportunity to continuously replenish and refine the model by identifying internal relationships between the indices without conducting extensive field and laboratory studies.

Conclusion. Based on the results of the work performed, the possibility of using direct spectral sensing to assess the state of soils both in direct contact and remotely was revealed. Multidimensional calibration allows us to find correlations between the forms of spectral characteristics and the chemical composition of the studied samples. The selection of the index format and the corresponding spectral bands for it is a necessary step in creating an MSS for monitoring the state of soils.

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Contribution of the authors:

T. V. Berdnikova — formulation of the purpose and objectives of the study, conducting the experiment, text preparation, formulation of the conclusions; V. V. Ermakov — scientific supervision, analysis of the research results, revision of the text, correction of the conclusions.