Colorimetric Parameters Modeling of Test Micro-Ecosystems for Lands Pollution Remote Sensing

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ABSTRACT

The paper describes a methodology of determining the toxicity sources, using bioassay based on the wildlife objects that change their colorimetric parameters under the influence of toxic factors. The work explores the dynamism of the colorimetric attributes associated with plant pigments. It can be determined by computer processing of the data obtained from digital remote sensing of the lands affected by toxic pollution by means of such relatively low-cost and straightforward methods as digital photography from an aircraft or a drone. The results obtained do not allow direct measurements but rather serve as a basis for the development and characterization of new biomarkers.

Keywords: pollution, system dynamics, colorimetric parameters, remote sensing.

INTRODUCTION

The toxicity of a surface run-off from the lands with man-made and settlement objects in many cases can become a source of various threats to biosafety. Urbanization of the modern world increases the likelihood of emerging sources of such threats in vast areas not entirely accessible for contact sensing. The use of digital photography from an aircraft provides the abilities for the implementation of these sources’ detection.

Pollution of the natural environment, for example, during hydrocarbon field exploitation, is related to various stages of the technological processes of oil and gas production and processing. The greatest danger of penetrating toxicants into natural landscapes arises during drilling of wells, transportation of extracted fluids, and exploitation of deep disposal and water dump wells in emergencies. All the components of landscapes, from plants to groundwater, are being polluted. The most significant load is imposed by the soils lying
on the way of technogenic streams. In a soil profile, the systems of contrast geochemical barriers are formed on which soluble salts and heavy metals accumulate, sometimes in ecologically critical concentrations [Vysotskaya, 2016]. Stormwater run-offs in cities are an essential source of pollution of the coastal sea area, because they include chemical compounds the concentration of which exceeds MPC [Beliaeva, 2012].

A bioassay with the usage of wildlife objects that change their color (colorimetric parameters) under the influence of toxic factors of the technogenic environment is employed to determine the sources of toxicity. A biofilm of microalgae formed on the solid pavement (asphalt, concrete, etc.) of the areas on the bottom of small temporary reservoirs (puddles) arising after rain, in many cases, are suitable for the role of biological test object [Bykh, 2016]. When the biofilm is not formed, an artificial microalgae biofilm full-grown on artificial substratum plates can be used. Such biofilm is the simplest version of a test micro-ecosystem (TMES). Such TMESs can be placed into small reservoirs, which surface run-offs flow into, using ground-based methods or dropped from an aircraft in special descent vehicles. The availability of toxicity in the aquatic environment can be remotely recorded by the computer analysis of the RGB-model of digital snapshots of microalgae biofilms. The conditions of TMESs are used for receiving the information necessary for remote sensing of toxicity in a surface run-off. In this regard, the following problem arises: it is necessary to optimize the colorimetric parameters of these conditions to minimize the time period for sensing and the number of aircraft departures.

When addressing the problem, the two circumstances should be taken into account:

- a high degree of measurement quality of the colorimetric parameters of TMESs can be provided in a much more comfortable manner at the stage of TMESs preparation under laboratory conditions than after placing them (after dropping from an aircraft) at the places for detection of toxicity’s availability or absence (after this – “in the field environment”);
- in the field environment, the nature of dynamism of colorimetric parameters, and, correspondingly, the influence of toxicity on this dynamism, can be determined easier than the static values of these parameters. It is therefore appropriate, under the field conditions, to dispose of the TMESs that are at the most dynamical, regarding the changes in colorimetric parameters, stage of their development (succession) for remote sensing of toxicity.

Because of these two circumstances, it is needed to describe the regular (toxicity free) dynamics of the colorimetric parameters of TMES targeted at the identification of the phases of the cycle of this dynamics, for which the most visible and, respectively, suitable for remote sensing of toxicity changes exhibited in these parameters. Such a description can be carried out in the most appropriate manner based on the actual data obtained under laboratory conditions. Under laboratory conditions, it is also appropriate to prepare for the placement of TMESs under the field conditions at the most dynamic stage of changes in their states in the course of succession. Earlier, they used mathematical analysis of the RGB-model of digital images to describe the structure of relationships and the cycle of changes in the colorimetric parameters of similar biological communities. It is a formalized description based on a new mathematical model class – discrete models of dynamical systems (DMDS). These mathematical models were earlier applied to describe different nature systems [Nosov 2017, Nosov 2015, Vysotskaya 2016, Zholtkevych 2013, Zholtkevych 2018], including plant communities [Balyym, 2017]. DMDS models enable, based on the correlation matrix between the system components, to describe the structure of the system inter-component and intra-component relationships. The ineter-component relationships include all possible combinations of positive, negative, and neutral influences between any two components. The intra-component relationships can be only symmetric, that is “plus-plus”, “minus-minus”, and “zero-zero”. The structure of relationships in convenient form can be represented as a matrix or weighted graph. An idealized trajectory of the system (ITS) can be computed for given initial conditions using this relationship structure. The ITS reflects the cycle of changes in the values of system components (in conditional scores).

The anthropogenic influence in limnological systems using remote sensing methods provides:

- Selection of remote sensing data, cartographic materials, and descriptive information;
• Creation of a detailed digital map of lake water area and coasts using ultra-high-resolution remote sensing data;
• Determination of seasonal variability of the lake using time-varying images;
• Conducting the classification of the coastal territory to determine coastal vegetation and anthropogenic impact on water object;
• Determination of the sources of anthropogenic influence;
• Classification of aquatic vegetation;
• Determination of the lake temperature regime using time-sensitive images in the thermal channel;
• Measurements on the ground and water surface, test areas selection;
• Comparison and calibration of the results using remote sensing data processing and above-ground measurements;
• Creation of limnological system geodatabase.

In order to increase the monitoring efficiency using remote sensing data, there is a need to create the base of space images. This enabled to research the dynamics of the environmental parameters.

High-resolution images such as Spot, GeoEye, DigitalGlobe, Sich-2 with various ranges were used to analyze the man-caused impact on the water areas of the listed lakes and their coastal zones. Selection of remote sensing data, cartographic materials, and descriptive information was performed. The eutrophication effect analysis using space images processing methods is based on diffuse reflection coefficient of light by surface and subsurface water layers variation analysis. Coefficient changes when the concentration of phytoplankton increases. This, in turn, causes a diffuse reflection of light due to increased light scattering back to microalgae. On the other hand, this process is accompanied by increasing the content of phytoplankton pigments that absorb light intensively in specific intervals. This process leads to a decrease in the diffuse reflection of light in some regions of the spectrum. It should be taken into account during remote monitoring for different periods of the year. For the absorption processes, the skin-effect impact was considered. It leads to a decrease in the electromagnetic waves depth penetration into the thickness of the conductive environment.

The main periods of limnological objects seasonal variability were identified due to time-dependent remote sensing data analysis. In particular, it was discovered that there is an active reproduction of phytoplankton and algae in most lakes in the warm period of the year. During the cold season, water has maximum transparency, and algae are falling to the bottom. Therefore, for aquatic vegetation monitoring, remote sensing data should be used for summer (July – August). The depth definition measurement needs images for October and November [Zagorodnia, 2018].

The processes of reservoirs eutrophication are contaminated wastewatersreset, washing out and weathering of specific substances from soils, washing out of organic and inorganic fertilizers from agricultural land surfaces, and washing out of manure from farms, subsidence contaminations from the atmosphere.

The course of the eutrophication process takes place in several successive stages. At the first stage, there is an accumulation of nitrogen or phosphorus minerals in the water. This process is usually short. In the future, there is intensive algae growth. As a result, phytoplankton biomass, water turbidity, and oxygen concentration in the water’s upper layers are increased. One of the aquatic ecosystem’s eutrophication consequences is an increase of the blue-green algae growth intensity, which significantly reduces the indicators of water availability for drinking (bad smell and taste) as well as recreational purposes (swimming, bathing, fishing). Such water is allergenic and toxic. The metabolites of blue-green algae are sources of many diseases among fish and warm-blooded animals. The next step is complete oxygen disappearance in the water object depths. Afterwards, the processes of anaerobic fermentation begin [Greben 2018a, Greben 2018b].

Algae begin to die and gradually disappear; there are processes of bottom sludge intensive sedimentation. In the structure of these sludges, there is a high content of organic matter. Due to the occurrence of such processes, there are changes in the zoocenosis. The development of the blue-green algae is also a significant negative factor for the zoological diversity of aquatic ecosystems. Zooplankton is a natural filtrate, which usually absorbs small algae, and when the processes of reservoirs “flowering” occur, the colonial forms, which are practically not absorbed by zooplankton, developing. They become members of the trophic chain only after interacting with destroying them bacteria. The diversity of zooplankton in the direction of community
simplification diminishes. Small species begin to prevail, but they cannot destroy organic matter with the same intensity.

After the blue-green algae, death toxins of particular importance are formed because they have a wide range of biological effects and affect animals and people’s central nervous system.

A separate contamination factor for water ecosystems is the washing out of manure from farms and fields (for example, their concentration is approximately 100 times higher than the rates of wastewater cleaned by treatment facilities).

The pollution of reservoirs is judged by the change in their properties and composition under the influence of direct or indirect human activity and, as a result of such activity, became unsuitable for at least one type of water usage. Deterioration of the water quality indicators due to the changes in their organoleptic properties and the appearance of harmful substances is a direct criterion of aquatic ecosystems pollution.

A unique role is played by microorganisms (or bacteria) because they may change to adapt and transform the previously unknown organic compounds. Such compounds are synthesized today, and as a result of their use in human life, they enter the reservoirs, infecting the hydrosphere and living organisms.

Let us consider the most important consequences of the further occurrence of water ecosystems pollution processes. Polyphosphates are hydrolyzed to orthophosphates, and the bulk of soluble organic phosphorus-containing compounds are converted into orthophosphates as a result of the biological decomposition of organic matter.

Weighed phosphorus substances are usually understood as organic phosphates, but this group may also include chemically precipitated orthophosphates and biologically bound polyphosphates. The composition of phosphates in the suspended matter is usually not very interesting because the suspended matter is separated from water by means of the methods, which are selective concerning not the particles, but their size, charge, density, etc. Orthophosphates – with two or three exceptions, are the only salts of phosphoric acid found in nature. They are also the only salts of phosphoric acid currently used in fertilizers. Polyphosphates are polymers of phosphates, the chain of which passes between other chemical groups. This type of polymerization is known as the condensation reaction. Phosphate bonds are usually high-energy covalent bonds, which means that energy is released by breaking these bonds spontaneously or as a result of enzymatic catalysis. All phosphate fertilizers can be divided into three groups in terms of water solubility:

1) soluble in water (any crops easily digest them);
2) insoluble in water, but soluble in weak acids (including organic acids, available for plants);
3) insoluble in water and poorly soluble in weak acids (phosphates which are not digested by the vast majority of cultures, provided that acidic soils do not decompose these compounds with the appearance of more easily soluble salts).

The influence of the sodium and potassium components of mineral fertilizers on the vital activity processes of reservoirs is approximately the same as for phosphorus components. Therefore, observation of their incidences is also significant.

Comprehensive environmental assessment has to be based on environmental monitoring data analysis. For the general pattern, it is appropriate to use the remote sensing technologies and the methods of statistical analysis. It is necessary to diversify statistical information annually and seasonally. The authors propose using the correlation analysis tools to identify the interdependencies of the pollution parameters. This approach makes it possible to determine the critical factors and classify the sources of anthropogenic impact on the degree of danger.

“Window-method” is used to describe the dynamics of changes and determine the relationship between different components of anthropogenic impact. The correlation coefficient is calculated for each measurement with a limited number of neighboring measurements for each process. Thus, the dynamics of relationship intensity can be analyzed.

Building and using powerful information technologies can provide speed, visibility, and completeness of obtaining environmental information. When using such technologies, it is necessary to determine the possible approaches to address such issues as improving the land monitoring system, optimizing the sampling stations on anthropogenic soil contaminant location, and improving the quality and speed of anthropogenic impact influence and parameters of soil quality mapping.

According to the experimental research, the humus content in soil is associated with its spectral brightness. With the increase of humus in the soil, the spectral brightness of coefficients
decreases. The greatest optical difference between the humus-rich soils and the soils with low humus content is observed in the near-infrared spectrum (0.75–1.3μm).

A mathematical model of forecasting the groundwater level changes in an aquifer with the level fluctuations in water receiver on conditions of three-ply water-bearing layer allows making a reliable assessment and the forecast on flood level of a sloping hill which, in turn, allows making a prompt managerial nature-green decision on the provision of territory with the necessary level of environmental safety. The estimation of individual risk on the built-over flooded territories by considering the sloping hills was improved.

METHODS

The work aimed to find the colorimetric parameters dynamics cycle phases regarding the version of TMESs, for which the changes in the values of parameters are the most significant. Such changes allow distinguishing the TMES remotely performed under non-toxic conditions from the TMES affected by toxic effects, such as a surface run-off. The research task is to build the DMDS model to recover the phases of the dynamical cycle of the TMES colorimetric parameters.

The initial data for mathematical modeling was obtained by digital photography of the TMESs. The TMES units have plastic plates of a size of 40x50 mm, with the biofilm of a wild microalgae culture on the working surface. TMESs were placed in transparent plastic vessels of a volume of 2 liters filled with rainwater and bottom sediments from temporary rain reservoirs. Copper sulfate CuSO₄ was added to the vessels in the experimental series for producing the concentration of 0.05 mg/l that does not kill algae but suppresses their development. The experimental and control series included 12 vessels placed on a concrete surface under natural sunlight.

The initial data of the system colorimetric components to be modeled were obtained by computer processing of digital images. Each image was divided into segments, and the averages of the red (R), green (G), and blue (B) components of the segments were calculated. The Matlab package (with Image Processing Toolbox) was used for calculation. The component values related to different attributes of the system were calculated using the initial data. These components were the following: G/(R+G+B) – reflects the performance of the system determined by the amount of chlorophyll, R/G – pigment diversity, (R+G)/(R+G+B) – total biomass of live and dead algal cells.

RESULTS

As a result of mathematical modeling with the use of DMDS, idealized system trajectories for the control and experimental series of the TMESs were obtained. The trajectories show the cycle of changes in the values of the components of the system introduced above, hereinafter referred to as “colorimetric” ((G/(R+G+B), R/G, and (R+G)/(R+G+B)), and the fourth component explained below. The fourth component, hereinafter referred to as “latent”, does not have a specific physical or biological meaning and was introduced in the following way. In the Spearman correlation matrix between components, the coefficients of latent and colorimetric components’ were assumed to be equal to 0 (Table 1 and 2).

- The maximum values of the components of the ITS are highlighted in bold.
- The maximum values of the components of the ITS are highlighted in bold.

In the framework of our study concept, upon building the DMDS model, this zero-valued correlation can mean, along with the lack of relations between the latent component and one of the colorimetric components, also a two-way relationship of the “plus-minus” type. Such relationships play an essential role in maintaining homeostasis (dynamic equilibrium) in systems of different nature [Nosov 2015, Vysotskaya 2016].

Consider the ITS view built for the control series of TMESs, shown in Fig. 1. In Z-axis: values of the components of the system in conditional scores (1 – low, 2 – moderate, 3 – high); in horizontal axis: time moments.

Focusing on the parts of the ITS having the following features:

- the parts with relatively statical values of the colorimetric components. Therefore, such parts are useless for remote diagnostics because the statical colorimetric characteristics of a microalga biofilm can be associated with
the lethal effect of acute toxicity agents on microalgae (these parts will be conventionally called “statical”);

- the parts with the marked dynamism of colorimetric parameters can be caused only by processes in the living algal community containing organisms not killed by toxicants (such parts are referred to as “dynamical”).

The role of the dynamism of the colorimetric parameters of TMESs is related to the greater convenience of their use comparing to the static parameters for remote detection of changes in colorimetric parameters of a microalgae biofilm by digital photography. Regarding the possibility of conducting measurements according to digital photography and subsequent biological interpretation, the static and dynamic parts have to be selected in the first place concerning the values of G/(R+G+B) related to bio productivity and the values of R/G related to pigment diversity.

It is necessary to select the static part (time moments from third to sixth) and the dynamic part (from the tenth through third inclusive) on ITS for the control series. At the beginning of the dynamic part (10th, 11th, first moments), the R/G decreases, followed by an increase in the G/(R+G+B) (1st, 2nd, 3d moments). This dynamism has the following biological sense. The condition for the growth of the algal community productivity corresponds to the increase of the G/(R+G+B) values. It prevents the delivery of nutrients for photautotrophs into the water due to the decomposition of dead cells. In these cells, yellow-orange pigments prevail over green chlorophyll that causes high values of R/G. Such changes in the colorimetric parameters in the ITS dynamical part that is sensitive to biological factors allows suggesting a basic outline for the use of TMESs. It assumes the placement of TMESs into the field environment when features of the first half of the dynamical part arise (distinguished by decreasing of the R/G). It is followed by detection of the absence of toxicity along with an increase in the G/(R+G+B), or the presence of toxicity without the increase in the G/(R+G+B). In order to distinguish the absence of toxicity from such its concentration, when all living organisms in a TMES are being killed and, for some period, there is no dynamism in plant pigments, a diagnostic algorithm is needed.

The algorithm is also suitable for the cases when the toxicity agents do not kill algae and other living organisms of a TMES, but only decelerate their development.

As mentioned above, the idealized trajectory of the system affected by the toxicity of CuSO₄ with the concentration capable only of decreasing the development of aquatic organisms, but not killing them, is shown in Table 2. The view of the trajectory is a basis for the suitability of the algorithm for distinguishing two cases.

On the ITS presented in Table 2, a few stable and dynamical parts can be identified, but there

Table 1. The idealized trajectory of the system presents the cycle of changes in the colorimetric and latent characteristics of the times in the control series.

| Characteristic type | System components values (in conditional scores 1 – low, 2 – middle, 3 – high) |
|---------------------|----------------------------------------------------------------------------------|
| G/(R+G+B)           | 1 2 3 3 3 3 3 3 3 3 3 2 1 1                                                   |
| R/G                 | 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1                                                  |
| (R+G)/(R+G+B)       | 1 1 1 2 3 3 3 3 2 1 1 1 1 1 1                                                |
| Latent component    | 1 2 2 1 1 1 1 1 1 1 1 1 1 1 1                                                |
| Numbers of time moments | 1 2 3 4 5 6 7 8 9 10 11 11 11 11 11 11                                      |

Table 2. The idealized trajectory of the system represents the cycle of changes in the colorimetric and latent characteristics of the TMES in the experimental series.

| Characteristic type | System components values (in conditional scores 1 – low, 2 – middle, 3 – high) |
|---------------------|----------------------------------------------------------------------------------|
| G/(R+G+B)           | 3 3 3 2 1 1 1 2 3 3 3 3 3 3 3 3                                               |
| R/G                 | 3 3 3 3 3 3 3 3 3 2 1 1 1 1 1 1                                                |
| (R+G)/(R+G+B)       | 1 2 2 1 1 1 1 2 3 3 3 2 1 1 1 1                                                |
| Latent component    | 1 2 3 3 3 2 1 1 1 1 1 1 1 1 1 1                                                |
| Numbers of time moments | 1 2 3 4 5 6 7 8 9 10 11 12 13 14                                            |
is no part where the growth of $G/(R+G+B)$ immediately comes after a decrease of the $R/G$. It is worth noticing the presence of significant fluctuations of the mentioned parameters in this version of a TMES.

The ITS view built for the experimental series of TMESs, shown in Fig. 2. In Z-axis: values of the components of the system in conditional scores (1 – low, 2 – moderate, 3 – high); in horizontal axis: time moments. On the ITS, several stable and dynamical parts can be identified, but there is no area where an increase of the $G/(R+G+B)$ immediately precedes the decrease in the $R/G$. It is worth noting that both the growth and decline of quite considerable values is meant – in the range of fluctuations from the maximum to the minimum values observed in this version of TMESs.

Figures 1 and 2 show a significant difference between the dynamics of colorimetric components in the control and experimental series. Within this research scope, we will first be interested in the differences observed in the parts of ITS with the increase of the component $(R+G)/(R+G+B)$. It refers to the growth of this component which corresponds to the growth of biomass of microscopic algae. The increase in the area occupied by the biofilm of microscopic algae on the substrate corresponds to the biomass growth. An increase in the area can be easily detected by an appropriate analysis of CPs of digital images.

A meaningful biological interpretation can be given to the mentioned difference:

- in the control series, biomass grows along with stable and high productivity, stable and low amount of pigment diversity, and stable state of the system as a whole;
- in the experimental series, biomass grows in parallel with the increase in productivity and the stable and high amount of pigment diversity and stable state of the system as a whole.

The study results highlighted some additional abilities for increasing the sensitivity of TMESs to the presence of toxicity agents in a surface run-off. We have in view TMESs, the central part of which is a biofilm of microalgae. Similar TMESs are easy in manufacturing and usage.

![Figure 1](image1.png)
Figure 1. Dynamics of colorimetric parameters in the control series.

![Figure 2](image2.png)
Figure 2. Dynamics of colorimetric parameters in the experimental series.
and relatively cheap under the conditions where technogenic disasters can generate threats to bio-safety related to the toxicity of a surface run-off. The afore-mentioned features of TMESs determine the practical significance of these abilities. The obtained results are of interest to theoretical ecology. They were caused by additional possibilities of the formalized description of the simplest aquatic ecosystems used in the remote censoring methods of toxicity sources.

CONCLUSIONS

The results of mathematical modeling using the DMDS model enable, in principle, to determine the features of a stage of TMESs development, at which their use for remote diagnostics of toxicity in a surface run-off is the most efficient. The dynamism of colorimetric characteristics plays the role of such features. The colorimetric characteristics are related to plant pigments and can be determined by computer processing of the original data obtained by such a relatively low-cost and straightforward method as digital photography from an aircraft. The results of mathematical modeling obtained in the framework of the paper do not enable to calculate the intervals of mentioned values of dynamical colorimetric parameters suitable for diagnostic procedures per se. Regarding specific conditions, the problem solution can be obtained using a database, including the data on the conditions as well as the corresponding static and dynamic colorimetric parameters used for bio testing biofilms of microalgae. Further studies based on the results of this paper may aim at the development of such a database.

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