# ГЕОЛОГІЧНА ІНФОРМАТИКА

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## DEVELOPMENT OF EFFECTIVE ALGORITHMS OF SURFACE WATER POLLUTION DIAGNOSTICATION

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***The paper presents the following algorithm for the diagnosis of pollution of water objects: the theoretical bases for diagnosing the characteristics of the deterioration of the water objects condition (occurrence of malfunctions) with the deviation of their parameters from the standard ones on the steady or close to the steady (quasi-steady) modes of pollution development and further assessment of the level of risk of occurrence of a dangerous situation, the approval of management decisions on liquidation or minimization of this pollution impact on the ecology of the water object.***

***The development of effective algorithms of pollution identification at the initial stages of pollution of water resources will enable an assessment of the nature and level of water pollution with the increasing number of chemicals associated with an increase of anthropogenic pressure on water objects. To simulate the processes occurring in the aquatic environment, it is proposed to use the geographic information system (GIS).***

***The conducted studies indicate that the borders of identification of the initial development of the process of pollution spreading (the occurrence of malfunction) is largely determined by the number of parameters that are measured in the process of diagnosis. The sensitivity of this diagnostic method for the majority of one-dimensional malfunctions is proved.***

***Keywords: water objects, diagnostics, monitoring, geo-information system, mathematical model.***

**Introduction.** Water quality is a characteristic of water composition and properties, which determines its suitability for a specific type of water use. According to the teachings of V.I. Vernadsky the basis of the modern system assessment of the water quality (drinking, sewage, surface and underground) should be the classifications which contain indicators and criteria of the water composition and its properties (physical, chemical, biological), which are collectively suitable for solving a wide range of problems, connected to the protection of water resources, their use and diversity of types of hydro-economic activities. Such a system must simultaneously answer environmental, hygienic and technological requirements. Very regrettably, today such a system does not exist, mostly because of the complexity of this interdisciplinary task [1].

In assessing the quality of natural waters, three approaches are usually used: physico-chemical, bacteriological and biological, each of which allows you to receive important information, and, when used all together, it is possible to evaluate the aquatic environment from ecological point of view [7].

*During physico-chemical evaluation of water quality* one determines its transparency, the concentration of suspended particles (turbidity), ionic composition, total mineralization, the presence of organic and nutrient substances, the concentration of dissolved gases, the active reaction of water (pH) and others. These abiotic characteristics are very important, but not sufficient for complete understanding of the aquatic ecosystem condition. More complete information on ecosystem response to pollution can be obtained by analyzing the qualitative and quantitative composition of hydrobionts, the presence or absence in their bodies of substances hazardous to their lives [5].

*Biological methods for assessing the quality of water* are based on the estimates of the responses of plankton, benthos, macrophytes and fishes to the appearance of chemical substances of mineral and organic origin in the aquatic environment. The level of pollution of water bodies is assessed by the presence or absence of organisms-indicators based on a comparison of species diversity, population size and biomass of the population of polluted and clean zones. During this comparison it is usual to use absolute values and indices of species diversity [6].

The method of assessing the quality of water (as the habitat of hydrobionts) by species composition and indicators of quantitative development of species-indicators and the structure of groups formed by them is called bioindication. Bioindicators of water quality are organisms, the presence, amount or specefics of the development of which are indicators of natural processes or anthropogenic impacts that change the composition and properties of water as a environment where they exist. With the composition of the flora and fauna of water bodies, the quantitative ratio of their individual representatives it is possible to judge on the degree and nature of pollution and the condition of aquatic ecosystems. The method of bioindication allows evaluating the efficiency of the purification facilities and the distribution of pollution during the transboundary relocation of toxic substances.

Diagnosing the state of water objects is not a trivial task. This is a complex dynamic process.

On any monitoring object (of diagnosis) parameters and characteristics that describe the state of this system change over time.

Under the object of diagnosis one should think about a system that meets two conditions. First, the system can be located in two mutually exclusive and distinct states ("workable" and "disable" that is it satisfies or does not meet certain quality criteria). Secondly, it is possible to define elements (blocks, subsystems), each of which is also characterized by states that can differ and which are determined by the results of inspections.

The diagnostic algorithm is a sequence of tests performed which are included into a diagnostic test and the rules for processing the results of the tests to obtain a diagnosis.

Diagnosis is information about the diagnostic object, which allows assessing the quality of the system or its "malfunction", that is to identify the cause of its non-compliance with certain quality criteria based on the analysis of diagnostic parameters or symptoms.

Symptom is a form of displaying the deviation of the diagnostic parameter from its permissible values.

In order to diagnose the processes taking place at the object of diagnostics (water object), it is necessary to evaluate the changes occurring in it, as well as to predict these changes in conditions of uncertainty and to take effective managerial decisions for them. In addition, changing the parameters of the water system of one level of the hierarchy can appear (affect) due to the change of completely different characteristics of the water system of the second level of the hierarchy.

In the process of searching for new effective methods for diagnosing the status of water resources, it is first of all reasonable to develop algorithms for diagnosing water objects in quasi-steady regimes, when the process of the pollution of the water environment is just starting with some pollutant (malfunction), which worsens the state of a certain water object.

The purpose of the work is to develop theoretical foundations for identifying the characteristics of the deterioration of the state (faults) of water objects with the deviation of their parameters from the "standard" on the steady or close to the steady (quasi-steady) modes of pollution development and further assessment of the level of risk of a dangerous situation, taking management decisions on liquidation or minimization of this pollution impact on the ecology of a water facility.

**Analysis of recent research and publications.** An important contribution to solving the problem of water quality assessment, drinking water supply at the state level was made by such scientists as A.V. Jacyk, A.M. Tugai, V.J. Melnik, A.K. Zapolsky and many others. The issue of drinking water supply in certain regions was investigated by M.A. Safonov, V.O. Orlov, A.F. Kiselev, V.D. Rud, N.V. Yanko and others. However, the current situation of the quality of water resources indicates the need for further research in this area and is relevant.

**Presentation of main material.** Ensuring citizens' security and protecting society is one of the most important functions of the state. Unfortunately, Ukraine is currently the most critical region in Europe with anthropogenic pressure, which is several times higher than the average European level [9].

On the territory of Ukraine almost all spectrum of dangerous natural phenomena and processes of hydrogeological and meteorological origin may arise. These include large floods, catastrophic flooding, large snowstorms and ice-colds, hurricanes, tornadoes, squall winds as well.

The end of XX – the beginning of the XXI century is marked by cataclysms that are partially related to the problem of surface water purity – the threat of massive gastric infections, deterioration of the quality of drinking water, reduced bioavailability of surface waters and their self-cleaning ability. Therefore, the problem of clean water in many countries of the world and particularly in Ukraine plays a central role in water protection activities and is very relevant.

The realities of the today's Ukraine have led to the deterioration of the quality of water and the mode of river flow; have turned many rivers into cannels and a network of reservoirs and ponds. The development of effective algorithms for pollution recognition at the initial stages of pollution of water resources will enable an assessment of the nature and level of pollution of water with the increasing number of chemicals associated with an increase of anthropogenic pressure on water objects.

In the general case a linear mathematical model of an object of study with the presence of measurement errors can be represented by matrix equations of two types [10]:

$$\overline{Y_з} = A\overline{X} + \Delta\overline{Y_з} \quad (1)$$

or

$$\overline{W_з} = A\overline{X} + \Delta\overline{W_з},\ \ \overline{W_з} = \overline{Y_з} - T\overline{S_з},\ \ \overline{\Delta W_з} = \Delta\overline{Y_з} - T\Delta\overline{S_з}, \quad (2)$$

where $\overline{Y_з}$ – vector of relative deviations of parameters of the mode of operation of the object of study of dimension $(m\times 1)$; $\overline{X}$ – vector of relative deviations of the required parameters of the condition of the researched object, control and effects of disturbances of dimension $(n\times 1)$; $A$ – matrix of coefficients of influence of dimension $(m\times n)$; $\overline{S}$ – vector of relative measured perturbing and controlling affects, if they are not relocated into vector $\overline{Y}$ by means of transformation for a given structure of equations. The dimension of the vector $(\nu_з\times 1)$; $T$ – matrix of coefficients of dimension influence $(m\times \nu_з)$.

The diagnostic model of the studied object of the type (1) is correct to use in the following conditions:

- the diagnostic model takes into account the program of management of the investigated object in the diagnostic mode. In this case if the control affects are measured, then they are introduced into the vector $Y_з$, if not measured then they are absent; the deviation of the control parameters is equal to zero;
- there is no rejection of perturbation effects in the diagnostic mode;
- there are no errors in measurements of perturbation effects;
- the characteristics of the reference modules correspond to the nominal characteristics or the identification of the mathematical model with the individual characteristics of the investigated object (phenomenon) is performed, that is, there is no influence on the vector $Y_з$ of natural dispersion of the characteristics of the modules of the object (phenomenon);
- there is no reduction of the measured parameters to the standard atmospheric conditions. In the opposite case, when converted to standard atmospheric conditions, the components of the vector $Y_з$ will become correlated.

In all other cases, it is necessary to use a diagnostic model (2).

In real modeling conditions the object properties change in a wide range, therefore, in order to ensure the necessary efficiency of the diagnostic system, it is necessary to have a standard of controlled parameters and a matrix of affecting factors at each diagnostic mode for each thematic layer of the system in the appropriate conditions of the study (diagnosis). For this purpose, it is best to use a comprehensive GIS [3]. However, today, the fully-variable multifunctional mathematical model of GIS with all thematic layers in the memory of a computer is not possible due to certain restrictions of these devices.

To diagnose quasi-stationary processes (phenomena) occurring on certain water objects, it is legitimate to use a mathematical model (1). To take into account the accuracy of the measurement of the parameters, the output system (1) is normalized by dividing each $i^{th}$ equation by the corresponding mean-square deviation $\sigma_i$ which is equivalent to the multiplication of the left matrix equation (1) on the diagonal matrix

$$\sum\nolimits_y^{-1} = \begin{vmatrix} \frac{1}{\sigma_{y_1}} & & & & & \\ & \cdot & & & & \\ & & \cdot & & & \\ & & & \cdot & & \\ & & & & \cdot & \\ & & & & & \frac{1}{\sigma_{y_m}} \end{vmatrix}. \quad (3)$$

After rationing and taking into account the measurement errors we:

$$Z_з = \hat{A}\overline{X} + \Delta\overline{Z}_з,\ \ \overline{Z}_з = \overline{Z} + \Delta\overline{Z}_з, \quad (4)$$

where

$$\overline{Z}_з = \sum\nolimits_y^{-1}\overline{Y}_з,\ \ \overline{Z} = \sum\nolimits_y^{-1}\overline{Y},\ \ \Delta\overline{Z}_з = \sum\nolimits_y^{-1}\Delta\overline{Y}_з,\ \ \hat{A} = \sum\nolimits_y^{-1}A. \quad (5)$$

Vector components $\Delta\bar{Z}_3$ are independent random variables distributed under normal law with zero mathematical expectations and dispersions that are equal to 1, that is

$$Z\left(\Delta\bar{Z}_j\right)=N(0,1),\quad \operatorname{cov}\left(\bar{Z}_i,\bar{Z}_j\right)_{i\neq j}=0. \qquad (6)$$

While solving the task of diagnosing of water resources condition it is possible to have 2 different situations:

– number of parameters of condition which will be reflected in the measured vector $\bar{Z}_3$, less than matrix rank $\hat{A}(r\le n)$. In this case to each combination $C_m^{\nu}$ $\nu=\overline{1,(r-1)}$ of parameters one can put matchable image and solve the task on the basis of theory of images recognition [8];

– number of parameters of technical condition which will be reflected in vector $\bar{Z}_3$, is equal or is of higher rank vs $\hat{A}$ matrix rank. In this case, any combination of parameters of condition $C_m^{\nu}$ $\nu=\overline{n,m}$ will correspond to the entire space of controlled parameters that makes the task unsolvable.

At the same time at the first stage the check of the hypothesis of belonging of the vector with measured parameters to the image of the considered malfunction should be conducted. It is done with the help of the probability estimation criterion. And at the second stage the solution is made only of those subsystems, which, with a given probability (0,95), explain the deviation of the vector of the measured parameters [2].

In order to diagnose the condition of water objects, the probability of simultaneous occurrence of less number of malfunctions is higher than the probability of simultaneous occurrence of a greater number of malfunctions; therefore the task of diagnosing a natural or anthropogenic system is appropriate to be solved by consistent testing of hypotheses with increasing number of malfunctions [4].

In the study of one-dimensional continuous failures the system of equations (1) are converted into a system with one variable, that is, the vector $\bar{X}$ is converted into a scalar $\bar{x}_j$:

$$\bar{Z}_j=\hat{A}_j\bar{x}_j,\quad \bar{Z}_3=\bar{Z}_j+\Delta\bar{Z}_3,\quad \bar{Z}_3=\hat{A}_j\bar{x}_j+\Delta\bar{Z}_3, \qquad (7)$$

where $\hat{A}$ – $j^{th}$ column of matrix *A*.

During parameter of technical condition change from $-\infty$ to $+\infty$ the vector $\bar{Z}_j$ varying in size and direction will lie on the straight line, whose position in the space of controlled parameters can be assigned by the vector $\hat{A}_j$ (putting $\bar{x}_j=1$); that is the images of one-dimensional continuous failures in the space of armed controlled parameters are straight lines passing through the origin of the coordinates. Because of the noisiness of the vector of substitutable parameters the system of equations (7) is incompatible. The degree of incompatibility can be judged by the square $J_j$ of the perpendicular $L_j$, which is pulled down from the end of the vector $\bar{Z}_3$ to the vector $\hat{A}_j$ (Fig. 1).

If the vector of substitutable parameters $\bar{Z}_3$ is a reflection (cause) of $j^{th}$ malfunction and on this reflection the errors of measurements of the measured parameters of the controlled parameters are imposed, the system of equations (7) is compatible and the square $J_j$ of the perpendicular $L_j$ will depend only on the measurement errors:

$$J_j=L_j^TL_j=\bar{Z}_3^TB_K\bar{Z}_3, \qquad (8)$$

де $B_K=I_m-\dfrac{\hat{A}_j\hat{A}_j^T}{\hat{A}_j^T\hat{A}_j}$.

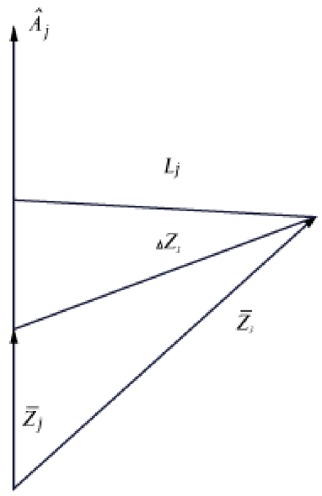

**Fig. 1. Graphic interpretation of equation system incompatibility (7) due to noisiness of vector**

Taking into account the errors of measurement that were reflected in vector $\bar{Z}_j$, we will get the amount of information that can be distinguished in the following way:

$$\hat{J}_j=\Delta\bar{Z}_3^TB_j\Delta\bar{Z}_3. \qquad (9)$$

As shown in the work [9] the properties of matrix $B_j$ and component of vector $\Delta\bar{Z}_3$ are such that quadratic form (9) is divided according to law xi-square with $m-1$ degrees of freedom.

$$Z\left(J_j\right)=\chi^2(m-1). \qquad (10)$$

For a given probability of identification error α and vector length $\bar{Z}_3$ one can determine the quantile of the distribution $J_{1-\alpha}$ [9]:

$$P\left\{J_j\le J_{1-\alpha}\right\}=1-\alpha. \qquad (11)$$

Thus the condition of vector $\bar{Z}$ belonging to $j^{th}$ malfunction (condition of compatibility) with probability $(m-\alpha)$ may be put in the following way

$$\tilde{J}_j=\frac{J_j}{J_{1-\alpha}}\le 1. \qquad (12)$$

Thus without solving the system of equation one can obtain the answer to the question whether the measured vector $\bar{Z}_3$ is the product of ion is the $j^{th}$ malfunction.

Then all compatible subsystems are solved. The solution for $j^{th}$ malfunction for which each condition (12) is fulfilled, is carried out according to the formula

$$x_j=\frac{Z_j^T\hat{A}_j}{\hat{A}_j^T\hat{A}_j}. \qquad (13)$$

In order to determine condition under which vector $\bar{Z}_3$ is a reflection of $j^{th}$ malfunction and will be incompatible with image of $k^{th}$ malfunction, it is necessary to pull down perpendicular $L_{jk}$ from the end of vector $\bar{Z}_3$ onto the image of $k^{th}$ malfunction. In this case the quadratic form

$$J_{jk}=L_{jk}^TL_{jk}, \qquad (14)$$

is split according to the law of xi-square with $(m-1)$ degrees of freedom and parameter of non-centrality $\lambda^2=\bar{Z}_3^TB_k\bar{Z}_3$ [10]. For a given probability of identification error α, with known accuracy of measurements of controlled parameters, it is possible for the given degree of malfunction $x_j$ development to find quantile of breakdown (distribution) $\left(J_{jk}\right)_{\alpha}$:

$$P\left\{J_{jk} \le \left(J_{jk}\right)_{\alpha}\right\} = \alpha \,. \quad (15)$$

Vector $\bar{Z}_з$ with probability $1-\alpha$ will not coincide with image of k$^{th}$ malfunction if quantile (15) will be higher than quantile $J_{1-\alpha}$ of breakdown (distribution) (15):

$$\left(J_{jk}\right)_{\alpha} > J_{1-\alpha} \,. \quad (16)$$

The smallest magnitude of malfunction $\bar{x}_j$ for which the correlation (16) is valid, will be searched border of diversity $j^{th}$ malfunction in given conditions of diagnosis.

For geometric interpretation of received results let's describe cylinder around image of malfunction $\hat{A}_j$, the surface of which is located at the distance $\sqrt{(J_j)_{1-\alpha}}$. Around the image of malfunction $\hat{A}_k$ the similar cylinder is located the borders of which are at distance $\sqrt{\left(J_{jk}\right)_{\alpha}} = \sqrt{\left(J_{jk}\right)_{1-\alpha}}$. The presence of accidental errors of measurement causes the situation when vector of errors $\Delta\bar{Z}_з$ might be rotated to any direction relatively to vector $\bar{Z}_j$ and is not dependent on the size and direction of vector $\bar{Z}_j$. Having designed the cylinders on the area created by images of $j^{th}$ and $k^{th}$ malfunction we will receive stripes along images of these malfunctions.

We will present the multidimensional space in which the vector $\bar{Z}_з$ is located on the area (square) as a circle with a center at the end of the vector $\bar{Z}_j$ and with radius $\sqrt{\left(J_j\right)_{1-\alpha}}$.

On this area we will consider a vector $\bar{Z}_{гр} = \bar{Z}_з$ characterizing one of the worst variants of the measurement and which is a reflection of this malfunction. The end of the vector $\bar{Z}_{гр}$ is on the border of $j^{th}$ malfunction and a circle. At the same time, various variants of the vector $\bar{Z}_{гр}$ location are possible.

Let us consider 3 typical cases. In image 2 vector $\bar{Z}_{гр}$ which is a reflection of $j^{th}$ malfunction will not differ from image $k^{th}$ malfunction, that is vector $\bar{Z}_{гр}$ being in the center of cylinders crossing, may be attributed both to $j^{th}$ and $k^{th}$ malfunction.

On Image 4 a limit case is represented.

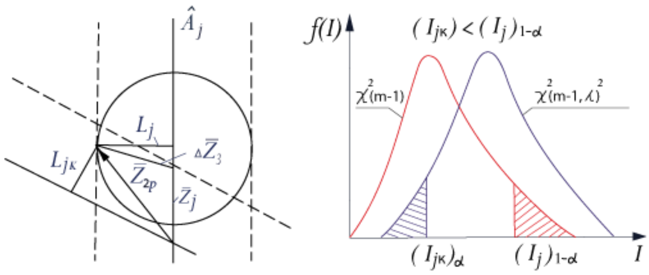


**Fig. 2. Graphic interpretation of the indistinguishability of two one-dimensional malfunctions**

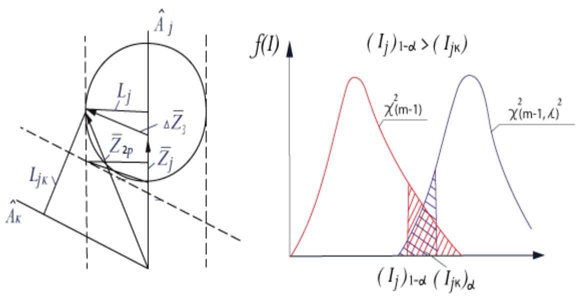


**Fig. 3. Graphic interpretation of measured parameters when relate only to $k^{th}$ malfunction**

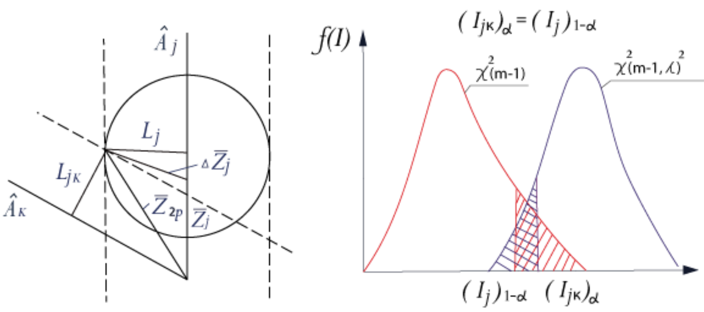


**Fig. 4. Graphic interpretation of limit case**

The magnitude of the malfunction $\bar{x}_j$ which determines the border of differentiation of $j^{th}$ malfunction when comparing it with $k^{th}$ malfunction for given conditions of diagnosis one can calculate with the formula (8)

$$\left|\bar{x}_j\right| = \frac{\sqrt{\psi(m,\alpha)}}{\left\|\hat{A}_j\right\| \cdot \left|\sin\left(\hat{A}_j, \hat{A}_k\right)\right|} \,.$$

**Conclusions.** The conducted studies indicate that the borders of identification of the initial development of the process of spreading pollution (occurrence of malfunction) are largely determined by a number of parameters that are measured in the process of diagnosis. However, an increase in the number of substitutable parameters for more than 10-12, in terms of malfunctioning, is inappropriate, since it can lead to a significant reduction of the recognition boundaries. Measure 8-10 of the most informative parameters leads to the fact that the borders of identification for majority of one-dimensional malfunctions will not exceed 1% of the degree of their development, which characterizes the sensitivity of this method of diagnosis.

However, the given algorithm, unfortunately, cannot provide an effective diagnosis of water objects for all situations, since many cases of water pollution (malfunctions) are more complex, that is, two- and more dimensional. In addition, it is required to have a number of researches of diagnosing of dynamic processes and phenomena occurring in certain areas.

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## РОЗРОБКА ЕФЕКТИВНИХ АЛГОРИТМІВ ДІАГНОСТУВАННЯ ЗАБРУДНЕНОСТІ ПОВЕРХНЕВИХ ВОД

***У роботі представлено алгоритм діагностування забруднення водних об'єктів. Розроблено теоретичні основи діагностування характеристик погіршення стану (виникнення несправностей) водних об'єктів при відхиленні їх параметрів від еталонних на сталих або близьких до сталих (квазісталих) режимах розвитку забруднення та наступної оцінки рівня ризику виникнення небезпечної ситуації, ухвалення управлінських рішень щодо ліквідації або мінімізації цього забруднення на екологію водного об'єкта.***

***Розробка ефективних алгоритмів розпізнавання забруднення на початкових етапах забруднення водних ресурсів дасть можливість оцінки характеру та рівня забрудненості вод зростаючою кількістю хімічних речовин, пов'язаних із посиленням антропогенного навантаження на водні об'єкти. Для моделювання процесів, що відбуваються у водному середовищі, пропонується використовувати геоінформаційну систему (ГІС).***

***Проведені дослідження свідчать, що границі розпізнавання початкового розвитку процесу поширення забруднення (виникнення несправності) багато в чому визначаються кількістю параметрів, що замірюються в процесі діагностування. Доведено чутливість даного методу діагностування для більшості одновимірних несправностей.***

***Ключові слова: водні об'єкти, діагностування, моніторинг, геоінформаційна система, математична модель.***

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## РАЗРАБОТКА ЭФФЕКТИВНЫХ АЛГОРИТМОВ ДИАГНОСТИКИ ЗАГРЯЗНЕННОСТИ ПОВЕРХНОСТНЫХ ВОД

***В работе представлен алгоритм диагностики загрязнения водных объектов. Разработаны теоретические основы диагностики характеристик ухудшения состояния (возникновение неисправностей) водных объектов, при отклонении их параметров от "исправных, эталонных" на стационарных или близких к стационарным (квазистационарных) режимах распространения загрязнения и последующей оценки возникновения опасной ситуации, принятие управленческих решений по ликвидации или минимизации распространения этого загрязнения на экологию водного объекта.***

***Разработка эффективных алгоритмов распознавания загрязнения на начальных этапах распространения загрязнения водных ресурсов даст возможность оценить характер и уровень загрязнения вод растущим количеством химических веществ, обусловленных усилением антропогенной нагрузки на водные объекты. Для моделирования процессов, происходящих в водной бреде, предлагается использовать геоинформационную систему (ГИС).***

***Проведенные исследования свидетельствуют, что границы распознавания начального развития процесса распространения загрязнения (отклонения от эталонного значения) во многом определяются количеством параметров, которые измеряются в процессе диагностирования. Показана чувствительность данного метода диагностирования для большинства одномерных неисправностей.***

***Ключевые слова: водные объекты, диагностирования, мониторинг, геоинформационная система, математическая модель.***