PhD Nemtsova A.A.[*], PhD Ponomarenko E.G.[**]

National University of Pharmacy, Ukraine[*]

O.M. Beketov National University of Urban Economy in Kharkiv, Ukraine[**]

Features of modeling as a method of scientific research in the field of environmental protection.

Modeling as a method of scientific research was formed in the middle of the nineteenth century. However, some of its elements we can found much earlier. In the works of ancient scientists, one can already find the terms "analog," "analogy," or "likeness", which underlie modern methods of modeling. Euclid was the first scientist who introduced the concept of an analogy. He regarded the analogy as a kind of relationship, representing a proportion. Thus, Euclid introduced the notion of a quantitative analogy. Later, Plato and Aristotle extended the concept of analogy to the most diverse areas of reality; in their works, they considered both quantitative and qualitative analogies. The main difference between them is that quantitative analogies imply the equality of relations, and qualitative analogies consider similarity as a similarity of functions.

The concept of analogy was widely used to penetrate the world that is inaccessible to immediate perception. For example,

- Democritus and Leucippus compared dust particles in the air with atoms;
- Ancient Roman scientist Strabo made a conclusion about the mobility of the earth's crust based on the analogy between the tides and ebbs of the sea and the breathing of living beings. He argued, "As living beings cleanse their bodies, so the sea throws all foreign bodies ashore, but if small islands can be flooded or raised to the surface, the continents can be raised or lowered in the same way."

Ancient scientists and philosophers have developed certain conditions for the legitimacy of analogs. Modern scientists also use these conditions today. For example, the analog and prototype should have as many essential common properties as possible for them. Analogies of the above type were harbingers of modern models based on similarity.

In the ancient world, the predecessors of another class of models, physical ones, also emerged. In ancient Egypt, often before building a large object, they made a small copy of it. Based on the results of the tests of this copy, they made a conclusion about the properties of the original.

Newton in his works has developed the logical foundations of modeling. His theorem on the similarity of motions allowed the results of research of one process to extend to all similar processes.

Thus, the elements necessary for the development of the modeling method (the conduct of analogies, the use of reduced copies, and the establishment of similarity of processes) gradually accumulated in the depths of natural science. In the middle of the nineteenth century, a qualitative change occurred, namely, the modeling took the form of a method of scientific research. The reason for this qualitative leap was the trend of the transition from the study of matter to the study of processes that appeared by this time, which is much more complicated. The difficulties involved in developing the theory of complex processes led scientists to look for new methods that would link empirical data to theory. Historically, mechanical models in physics have become the first type of models in natural science. Thus, modeling has deep roots. However, it is a young method of scientific research and it continues to develop.

Now, under the model, researchers understand a material or mentally imagined object that, in the process of studying, replaces the original object, preserving the main important characteristics typical for this study. For example,

- The architect designs a new building and builds it first from the cubes on the table. This model allows you to judge only the appearance of the original.
- The lecturer, explaining the functioning of the circulatory system, uses a poster with a schematic depiction of large and small blood circulation in the human body. This model allows you to better judge the movement of blood in the body than, for example, anatomical atlas.
- Test the aircraft in a wind tunnel. The wind tunnel is a model of airflows.

The variety of models used in scientific research caused the need for grouping them into classes. Now scientists use the following main classification characteristics of models: by implementation; by the nature of the temporal or spatial description; by the degree of definiteness of the forecast; by the nature of the description of spatial characteristics; by possible description of the dynamics of the process; and by appointment.

Classification of models by implementation is shown in Figure 1.

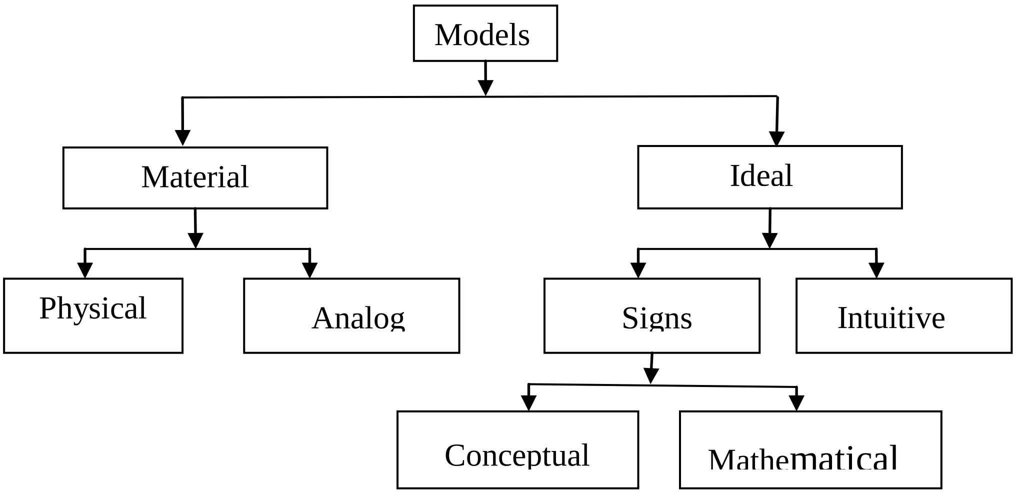

Fig. 1. Scheme of classification of models by implementation.

The material models are the material reflection of the original object (prototype). Such models are associated with the prototype geometric, physical and other characteristics. The research process in this case is connected with the material impact on the model and is of an experimental nature.

The physical models are an enlarged or reduced copy of a real object (prototype). For example, it may be an aquarium with its plant, animal and microbial world in ecology; artificial trays in hydrodynamics and hydraulics; models of buildings in architecture; a planetarium in astronomy etc. The main problem of physical modeling is the dissemination of the results of the study using the model to the real conditions of the prototype. For this, scientists use a special similarity theory, in which they formulate the similarity criteria and the rules for recounting the simulation results. For example, in hydrodynamics, as such similarity criteria, the conditions of equality of the Reynolds and Froude numbers for the model and the prototype are often used. This allows the recalculation of process time and dynamic characteristics. In the environment sciences the similarity criteria have not yet been developed, so ensuring reliability in using the simulation results on the conditions of a real ecosystem is a big problem. In this regard, the application of physical models in the environment is limited. The disadvantage of physical models is the complexity and high cost of their construction and operation

The analog models based on the analogy of processes and phenomena of different physical nature, but equally described formally. For example, heat transfer and mass transfer, mechanical and electrical vibrations.

The ideal models based on the mental analogy of the prototype and model. Such modeling, in contrast to material modeling, has a theoretical rather than an experimental character.

The intuitive models based on an intuitive notion of a prototype that cannot be formalized. For example, life experience is a model of the surrounding world. Intuitive models have found application mainly in the social sciences.

A sign models use sign transformations (diagrams, drawings, graphs, formulas). Such models must necessarily include a set of laws on which it is possible to operate with the chosen sign transformations.

The conceptual models based on a verbal description of the prototype. Usually such models have the form of graphs, diagrams, schemes of interaction between individual parameters of the model with an explanatory text. For example, in environmental sciences, these are schemes of the cycle of nitrogen, phosphorus, carbon in the aquatic ecosystem; schemes of food chains and so on. Typically, text, table or graphic material accompanies such block diagrams. Conceptual models have found wide application in environmental sciences, since they are the development of the tradition of a naturally scientific description. The purpose of conceptual models is to give a clear, generalized and sufficiently complete expression of knowledge and ideas about the object under study in the framework of a certain scientific concept. The advantage of conceptual models is their universality and visibility. Disadvantages of this class of models are their static, ambiguous interpretation, the inability to simulate various situations. Conceptual models are mandatory precursors of a more promising modern class of ideal models - mathematical models.

Mathematical models allow a researcher to describe a prototype using certain mathematical dependencies and expressions. Researchers use them mainly for the description of processes. For example, the dependence $S = v \cdot t$ is a model of uniform rectilinear motion.

Depending on the nature of the temporal or spatial description of the process, the models are of two types: discrete and continuous models. Discrete models describe a simulated process on a fixed sequence of time or spatial points. Continuous models allow the researcher to obtain the characteristics of the simulated process at any time or at any point in space.

Depending on the degree of certainty of the forecast, the models are divided into deterministic (cause-effect) and stochastic (probabilistic). Deterministic model are models in which the results of modeling are uniquely determined. Stochastic models are models that take into account the random nature of the process. These models allow obtaining only probabilistic characteristics of the process such as the mathematical expectation, the interval in which the characteristics of the process can vary and the distribution of probabilities in this interval, the standard deviation.

Depending on the nature of the description of spatial characteristics, the models are point or spatial. In the point models, in contrast to the spatial models, it is impossible to take into account the spatial characteristics of the modeling object. Researchers use models of varying complexity, depending on the need to detail the properties of the simulated process. For example, when studying the dynamics of biomass in an aquatic ecosystem, one can approach to various degrees of detail and, consequently, use models of varying complexity.

For small reservoirs with good mixing, researchers usually can neglect the uneven distribution of the main characteristics of the ecosystem (biomass, biogenic stocks, etc.) along the reservoir space. In this case, it is possible to average the main characteristics of the depth and area of the reservoir and take into account only the change in the characteristics of the ecosystem in time. This will be a point model of the form $f = f(t)$. For sufficiently deep ponds, one cannot ignore the heterogeneity in depth. In this case, we need to use a one-dimensional model of the form $f = f(t, z)$. In fine shallow water bodies, there is usually good mixing and uniformity in depth, but there may be a significant heterogeneity in the area of the water mirror. In this case, it is expedient to apply a two-dimensional spatial model of the form f = f(t, x, y). In the case where the inhomogeneity of the process cannot be neglected in any dimension, a three-dimensional spatial model of the form f = f(t, x, y, z) is used.

Depending on the ability of the model to describe the dynamics of the modeling process, the models can be static or dynamic. The static models, in contrast to the dynamic models, do not allow taking into account the change in the characteristics of the process over time. Researchers usually use such models to describe steady-state processes for medium- and long-term forecasting and planning purposes. They traditionally use dynamic models to describe unsteady-state processes for operational forecasting purposes.

By designation, mathematical models are divided into descriptive, optimization, gaming and simulation models. Descriptive models allow describe processes. With their help, researcher can make predictive calculations for different situations. Optimization models allow make purposeful process control. They always include one or more of descriptive models, control variables (control parameters), one or more objective functions, and a system of restrictions on changing control variables. The goal of optimization is to choose the best management strategy.

Consider in the most general form the structure of the simplest optimization model in the example of a model for managing the water quality in a river. In this case, the water quality is the object of modeling. For simplicity, we will evaluate the quality of water using a single indicator and denote by C the value of this indicator (for substances this is simply the concentration of this substance). The quality of water in the river depends on a several number of external influences and processes within the aquatic environment. The description of this dependence requires the use of one or more descriptive models. We denote the set of descriptive models by M. For simplicity, we assume that the set M consists of one model of the form

$$\boldsymbol{C(x)} = \boldsymbol{C}\left(\boldsymbol{C}_0, \boldsymbol{G}, \boldsymbol{Q}_{in}, \boldsymbol{C}_{in}, \boldsymbol{T}, \boldsymbol{Q}, \boldsymbol{V}, \boldsymbol{Q}_{ww}, \boldsymbol{C}_{ww}, \boldsymbol{x}\right); \qquad (1)$$

where C_0 is the initial concentration of the substance. G is the watercourse characteristics. Q_{in} and C_{in} are the flow rate and concentration of the substance in the tributaries. T is the water temperature. Q and V are the flow rate and flow velocity in the river. Q_{ww} and C_{ww} are the flow and concentration of the substance in wastewater; x is the distance from the initial point of the stream.

Thus, the quality of water in the river depends on a set of parameters, which we denote by X. $\boldsymbol{X} = \{\boldsymbol{C}_0, \boldsymbol{G}, \boldsymbol{Q}_{in}, \boldsymbol{C}_{in}, \boldsymbol{T}, \boldsymbol{Q}, \boldsymbol{V}, \boldsymbol{Q}_{ww}, \boldsymbol{C}_{ww}, \boldsymbol{x}\}$

The set X consists of two subsets. The first subset includes uncontrollable parameters, the value of which we cannot affect in any way. These include the initial concentration, the characteristics of the watercourse and tributaries, water temperature, hydraulic characteristics of flow. The second subset ($U \in X$) includes control parameters, the value of which we can purposefully change. To them in our case are the wastewater discharge and concentration of matter in the wastewater.

An integral part of any optimization task is the objective function. Depending on the formulation of the optimization problem, the objective function can be one (single optimization goal) or several (it is required to achieve several goals simultaneously). Depending on the desired result, optimization consists in finding such admissible values of the control parameters at which the maximum or minimum of the objective function is reached. In our case, the objective function $\Phi = \Phi$ (u) determines the dependence of the concentration of the substance on the set of control parameters Q_{ww} and C_{ww}. The purpose of optimization in our case is to improve the quality of water by reducing the concentration of pollutant, so we will look for a minimum of the objective function. The descriptive model M makes it possible to calculate the concentration of a substance for each set of values Q_{ww} and C_{ww}. of control parameters.

An important point in constructing an optimization model is the development of a system of constraints for control parameters. Usually, we can manage of the values control parameters only within certain limits. Therefore, only those that satisfy the formulated constraints (admissible controls) are chosen from the whole set of controls. In our case, the constraints can have the form

$$\boldsymbol{Q}_{ww\min} \le \boldsymbol{Q}_{ww} \le \boldsymbol{Q}_{ww\max} \qquad \boldsymbol{C}_{ww\min} \le \boldsymbol{C}_{ww} \le \boldsymbol{C}_{ww\max}$$

Depending on the type of the descriptive model M, the objective function Φ(u), and the constraint structure (linear or nonlinear), there are various methods for solving optimization problems. Usually when solving environmental problems, we are faced with the need to achieve several goals, sometimes contradictory.

Usually the solution of environmental problems requires achieving several goals, sometimes contradictory. In such cases, researchers use multicriteria optimization models. For example, to ensure the improvement of water quality with a minimum of costs for water protection measures and (or) providing navigation on the river, etc. The solution of multi criteria problems is much more complicated than single-criterion ones. In this case, the solution obtained is of a compromise nature.

Game models researchers use to describe conflict situations. In them, there are always participants with opposite interests, namely the person making the decision (PMD) and the opposing persons or factors. This is a more complex class of models, based on the mathematical theory of games. Classic examples of game models are computer and business training games. This class of models has become widespread in the entertainment industry, in education, in the military sphere.

Imitational models researchers use to describe the behavior of complex systems. The aim of simulation is to simulate the behavior of a complex system in different conditions with the help of a computer. Such models are implemented in the form of software packages. The complexity of the simulated processes determines the features of the simulation models.

- The mathematical model underlying any simulation model must reflect many relationships between elements, a variety of nonlinear constraints, contains a large number of parameters, that is, it is very complex. This leads to the absence of an analytical solution of such a system of equations.

- Since the role of random factors for complex systems is usually significant, as a rule, one cannot neglect their influence on the modeled process. Simulation models often have a stochastic character. This also causes the impossibility of an analytical solution.

- The development and operation of simulation models require the use of a large amount of initial information, statistical methods of its processing and other numerical methods for solving the system of equations.

- The use of simulation models is impossible without modern computer technologies.

Taken into account the complexity of the structure of the ecosystem and ecosystem processes, simulation modeling has become widespread in the environment.

Modeling of complex processes includes the following stages: statement of the problem, conceptualization (construction of a conceptual model), specification, development of a mathematical model, and directly carrying out calculations based on the constructed model.

At the stage of formulation of the problem, the researcher identifies a finite number of properties and processes that are most essential for solving the assigned task. For example, the researcher sets a task to determine the possibility of using a reservoir for drinking purposes after the construction of a hydroelectric power station on it. In this case, it is necessary to determine the main indicators by which the water quality will be assessed; the main factors affecting the hydrodynamic characteristics of the reservoir; basic physical characteristics of the reservoir (temperature), etc. As a result, the researcher makes a list of the factors that he will take into account in modeling.

At the stage of conceptualization, the researcher summarizes all the information about the process in the form of a complete and logically consistent conceptual model. He presents the results in a visual form (diagrams, figures, tables) with an explanatory text. For example, the conceptual model of a water ecosystem should include descriptions of its interaction with the external environment, the structure, composition and function of the ecosystem.

At the specification stage, the researcher solves the following problems: defines all the parameters and functions of the model; establishes a correspondence between the measured process properties and the parameters and unknowns of the model; specifies units and methods of measurement.

The construction of a mathematical model is the most difficult stage of modeling. It is iterative in character. The accuracy of the description of the simulated process and the number of factors taken into account are set at the stage of setting the problem, but the amount of initial information and the level of knowledge about the basic laws of the process determine the possibility of achieving them. Therefore, for a single object often develop a whole series of models of varying complexity. The basic stages of constructing a mathematical model are presented below.

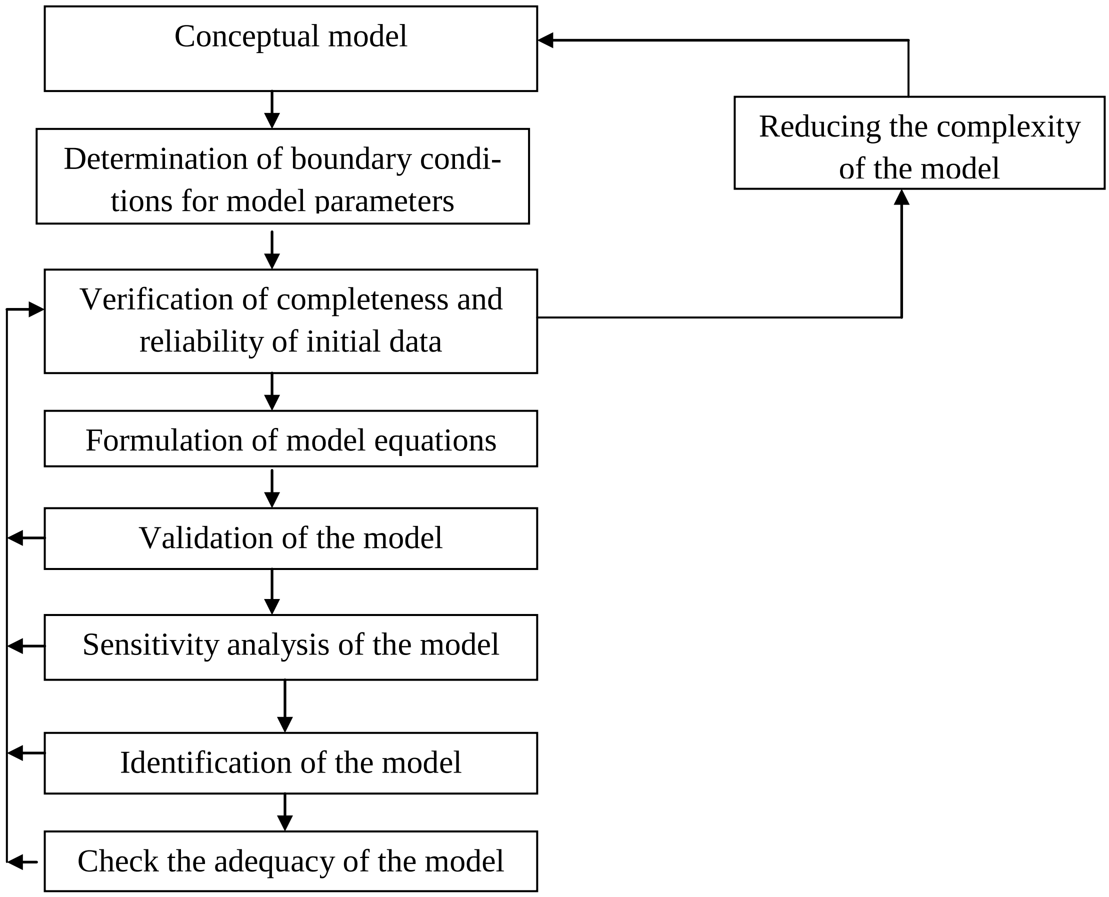

Fig. 2. Block diagram of the main stages of constructing a mathematical model.

Consider the basic stages of model construction on an example of development of mathematical model of quality of surface waters.

In the first two stages, the researcher analyzes the parameters included in the conceptual model and verifies the availability of the model with the original data. Parameters of the model can be universal constants (molecular weight, gas constants, gravitational constant, etc.) or serve as quantitative characteristics of certain processes in a water body (the rate of biochemical oxidation of the substance, flow velocity, etc.). Universal constants have exact numerical values. In the second case, only possible ranges of parameter changes can be set. If the initial data is not sufficient to determine all the parameters of the model, the conceptual model should be revised to reduce its complexity.

In the next stages of model development, the researcher formulates a model in the form of mathematical dependencies, analyzes its equations from the point of view of the ability to describe the simulated process and adjusts the model to real conditions.

Verification of the model consists in testing its internal logic. At this stage, we check: correctness of the reaction of the model to possible impacts, stability of the model for a long period and does the model take into account the fulfillment of the basic physical laws, for example, the law of conservation of mass and energy.

For example, for water bodies, the researcher analyzes the model's response to changes in external pollution sources, lighting conditions, hydrodynamic conditions, etc. Stability of the model means that there should be no accumulation of errors during long work with the model.

The sensitivity analysis of the model consists in studying the reaction of the model to the change in its parameters. If, with a slight change in the value of the parameter, there is a significant change in the results of the simulation, then the model is sensitive to this parameter. The values of such parameters should be determined during the adjustment of the model from the actual data (at the identification stage). If the simulation results depend little on the value of the parameter, then the model is insensitive to this parameter. Values of such parameters can be taken from literature data.

The identification of the model consists in determining the values of the model parameters from the field data. The identification criterion is the minimum deviation between simulation results and field data. By the magnitude of this deviation, using special criteria, for example, Fisher's criterion, judge whether the parameters are well chosen or not. If it is not possible to match the parameters so that there is a good match with the field data, then researcher can conclude that identification is impossible. In this case, researcher needs to look for a more complete array of initial data or change the conceptual model. The identification process indirectly takes into account the impact of those factors that are not included in the model, but have little effect on the simulated process. In the simplest case, model identification requires the use of the least-squares method, but for most models, the identification process requires the use of special methods or a selection procedure.

The verification of the adequacy of the model consists in testing it on the amount of initial data that does not coincide with the data for which it was identified.

A negative result at any stage of the simulation from verification to verification of adequacy requires refinement of the model parameters, increasing the amount of initial information or changing the conceptual model.

Complexity of ecological processes and processes of formation of surface waters generates a feature of the modeling methods used. These include field observations, full-scale and laboratory experiments, and mathematical modeling.

The method of field observations is historically the first method of research in ecology. He assumes the researcher's non-interference in the process and observation in natural conditions. The method has a passive and descriptive character. This method allows:

- to identify the main types of subsystems and their interrelationships;
- to determine the species composition of organisms;
- to give a description of the microclimate, soil type, hydrological regime, etc.;
- to determine the structure of the ecosystem at a qualitative level;
- to obtain quantitative estimates for the main indicators of the ecosystem, for example population density;
- to give quantitative estimates of some relationships, for example, the dependence of the intensity of photosynthesis on illumination, temperature, humidity, etc.;
- to provide a comprehensive description of the seasonal dynamics of individual components of the ecosystem.

The experimental method differs from the method of field observations by the active participation of the researcher in carrying out the experiment. The experiment always involves a deliberate change in external conditions. The technique used in this case is not important. For example, the study of the number of reindeer herds with the help of the newest means of tracking is still just an observation. A solution to the same problem, even with minimal technical means, but in conditions of isolation of predators, this is an experiment.

The method of carrying out an ecological experiment essentially depends on the level of control over the object under study and the number of variable factors. In a practically uncontrolled experiment, the experimenter produces a planned impact on the ecosystem, and then only monitors its dynamics. However, he cannot exclude natural external influences. An example of such an experiment is the experiment on the survival of deer in winter in a forest under conditions of additional feeding. In a practically controlled experiment, the experimenter can control external conditions throughout the experiment. For example, experiments on the reproduction of fish in aquariums. In a partially controlled experiment, the experimenter can control some external influences, but not all. For example, experiments on the dynamics of development of herd of deer in the conditions of the reserve. The experimenter can control feeding, the absence of poachers or predators, but does not control the weather conditions. Natural experiments are practically uncontrolled experiments, laboratory experiments are mainly partially controlled experiments. To provide practically controlled experiments, it is necessary to use very complex and expensive microcosmic installations that provide complete isolation of the research object from the environment.

The number of simultaneously changing factors determines the division into one-factor and multifactor experiments. The single-factor experiment corresponds to the classical scheme of conducting natural-science experiments. In a single-factor experiment, the experimenter studies the influence of one chosen factor on the process under study at fixed values of all other factors. This methodology proved to be quite effective in studying inanimate nature, especially in physics. However, in experiments with environmental objects that depend significantly on the entire complex of factors simultaneously, this approach is less effective.

Multifactor experiment corresponds to the scheme of carrying out the experiment, when the experimenter simultaneously changes all the factors affecting the process being studied. He produces a series of experiments in which not one but several factors change in each experiment. The values of these factors vary according to a special scheme, called the experimental design. The results of a series of experiments the researcher processes according to a special technique, which allows obtaining a multifactor description of the studied process as a function of several variables. Ronald Fisher developed the method of a multifactor experiment in the 30's of the 20th century as part of the theory of experimental design. This method proved to be very effective in environmental studies. For example, the noted Russian scientist ecologist Fedorov Vadim used this method to study the dependence of primary production on illumination, the content of nutrients and the composition of phytoplankton in a body of water. However, irrespective of the methodology of the experiment in the field of ecology, there is always a fundamental problem of transferring the experimental results to real conditions. A theoretically grounded and reliable solution to this problem is not yet available. Therefore, despite the fact that environmental experiments are poorly controlled, environmentalists prefer this kind of experiments.