NEW DIRECTIONS IN BIOPHYSICS OF AQUATIC ECOSYSTEMS

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Abstract. The paper presents new experimental and theoretical results of the study of the mechanisms of stability and controllability of communities of hydrobionts (microorganisms) in open aquatic ecosystems. The basis is the search and study of physicochemical mechanisms of action of density growth-controlling factors (DGCF) and the laws of sustainable coexistence of natural populations. Experimental and theoretical results were achieved: 1) elements of the mathematical theory of similarity of aquatic ecosystems are developed on the basis of joint environmental-hydrophysical equations of dynamics of their state in a dimensionless form: 2) the connection (theorem) of the maximum number of coexisting species (n) and the number of DGCF (m) is proved: $n < m$; 3) through the change of the input DGCF rules for the formation of a community structure with a predetermined species composition and methods for searching DGCF are proposed; 4) the fundamental phenomenon of autostabilization of the DGCF is revealed: independence of background levels of the DGCF from their input flows. The general environmental significance of the results is discussed in terms of the fundamental improvement of the predictive "strength" of mathematical models of aquatic ecosystems.

Key words: *ecosystem similarity, autostabilization, quantization theorem, coexistence principle, ecosystem models.*

1. INTRODUCTION.

It can be argued that biophysical ecology (i.e., the science concerned with studying the subject matter of ecology from the physical–mathematical point of view) is developing rather slowly. The rate of development of this science, which is highly important for developing scientifically based management of ecosystems and the biosphere, is limited by the following factors: (1) the absence of systematic experimental approaches (of the type used in physics) connected with the impossibility to make experiments with the ecological object which is unique (e.g., unique is the biosphere itself, a certain lake, river ecosystem, etc.); (2) the rare procedures for the verification of ecosystem mathematical models using field and/or experimental data; (3) the variety of interactions within ecosystems in terms of energy, matter, and control even for small-species communities; and (4) the absence of strict methods for the transfer of laboratory-scale experimental data to full scale. We shall discuss some solutions to the situation.

We shall consider water resources as an example. The rapidly increasing consumption of water will soon make the lack of freshwater a factor that will limit the development of civilization as severely as diminishing energy resources will do. As a rule, the interests of water users are conflicting. However, almost all of them pollute water environments, seriously interfering with ecosystems and making harmful alterations to them. Aquatic ecology must be able both to predict the environmental consequences of the activities of water users and also to satisfy their needs in the best possible way. The biophysics of ecosystems has three major branches with their own physical–mathematical methods: namely, (a) monitoring the integrated parameters of ecosystems, (b) the kinetic experimental approach, and (c) mathematical modeling, which is based on the first two branches. In its methodology, the biophysics of ecosystems currently tends towards reductionism, maybe because it has been used successfully in physical sciences. Investigations address the spatio-temporal distribution and dynamics of various ecological structures of aquatic ecosystems (species, age, sex, functional structure, and trophic structure) and the hydrochemical conditions of a water body. More specifically, the biophysics of ecosystems deals with:

— biochemical and population mechanisms: self-regulation of growth in aquatic communities, substrate consumption, material cycling, inter-specific relationships in the community;
— contribution of density and limiting factors to the stability of aquatic communities;
— physical principles underlying the theory of the search for limiting factors;
— laws of the stable coexistence of interacting populations;
— principles and theory of material cycling in aquatic communities;
— experiments, mechanisms, and the theory of migration behavior of aquatic organisms (plankton);
— scale-up of ecosystems;
— construction of ecosystems with tailored properties;
— ecosystems with closed material loops as models of biosphere-like systems.

The purpose of ecosystem biophysics is to reach such a level of knowledge about the elementary physical–biochemical mechanisms responsible for the functioning of aquatic ecosystems that would be sufficient to make valid prognoses of their natural and human-induced dynamics and to control their state.

A very important part of ecosystem biophysics is theoretical prediction of the development of aquatic ecosystems, including water quality. An instrument of prognosis (i.e., the theory and models of aquatic ecosystems) must be regarded as equal to the methods of biological monitoring [1], including remote control, and physicochemical analysis of the state of a water body. Until recently, modeling of aquatic ecosystems has been only (and rather weakly) related to data of the classical monitoring of water bodies. The existing procedure of model identification and verification (actually fitting to field data) does not allow an extrapolation of constructed models to other water bodies, because it disguises and mixes up the errors of measurements of ecosystem inputs and the lack of knowledge of mechanisms responsible for the functioning of ecosystems. The most serious drawback of the existing method of modeling aquatic ecosystems (compared with physics) is that modeling is unrelated to experimental investigations. Thus, we cannot gain any essentially new knowledge about the mechanisms of interactions of biological components, so the heuristic significance of investigations is limited. Experimental investigations are laboratory and/or semi-field investigations of both the kinetic characteristics of aquatic organisms and the behavior of a community in special experiments. Experimental methods in biophysical ecology must, like physical ones, provide insight into the internal structure of communities and interactions between populations. The deepest insight into the structure of an ecosystem, its parts and their functioning is gained when experimental and field data are coordinated and the logical consistency of this coordination can be verified by mathematical models of various hierarchical levels. Although biologists are sometimes skeptical about the achievements of mathematical modeling, this may be the only means to strictly verify ecological hypotheses, particularly in the case of events with multi-directional processes running simultaneously, and the universal method to check the ecological efficiency of different scenarios of controlling the state of a water body [2].

Contemporary knowledge of the structure of river, lake, and reservoir ecosystems and the practical positive control of the state of water bodies suggest more questions than answers. The answers are less profound than ecological problems. The reason is that aquatic ecology as a science encounters some objective difficulties related to the following sections (Sections 1.1−1.3).

1.1 Experiment in ecology.

In contrast to physics, ecology is poor in experimental approaches; we do not refer to methods of field observations but rather to experimental approaches similar to physical ones (i.e., a discriminating experiment with a whole ecosystem responding to a sole experimentally calibrated impact).

1.2 Complexity of ecosystems.

The rapid accumulation of ecological knowledge is naturally impeded by specific features of aquatic ecosystems. An ecosystem consists of numerous variously interrelated components, which are responsible for its counter-intuitive behavior (i.e., the behavior is opposite to what we can predict based on our limited knowledge, which seems to us quite complete). In ecology, this behavior has particularly grave consequences, as the human impact on aquatic ecosystems increases and there is rather limited time for thorough studies to counterbalance counter-intuitiveness. In this respect, physics has been in a better position for quite a long time. Counter-intuitive behavior can also be caused by changes in interactions between populations (due to adaptation, microevolution) that the ecology researcher is not aware of.

1.3 Non-trophic regulation of ecosystems.

In the general case, we adhere to classical concepts and assume that, to make a valid prognosis, it is sufficient to know only the trophic−energy structure of an aquatic ecosystem and to have basic knowledge of the species. However, an ecosystem comprises organized fluxes of energy, matter, and control. Processes of control may be even more important for a valid prognosis than material flows. Moreover, the effective specific mechanisms of regulation that have been selected in the course of long-term evolution and that include various (e.g., chemical) special signal systems can influence all species, from bacteria to humans. Thus, when we consider the impact of pollutants, we should study not only the processes of their decomposition and biochemical transformation but also their damaging effects on regulatory interactions and their interference with regulation, including communications.

2. FUNDAMENTALS OF WATER ECOSYSTEM: SIMILARITY THEORY.

If we address the problem of experimenting with real aquatic ecosystems, leaving aside quite successful experiments with water treatment facilities, we can see that a well-developed methodology is still lacking. There is an approach based on the construction of various sizes of experimental micro-ecosystems; there are systems of continuous cultivation of microorganisms, and finally there are test-tank or aquarium-type laboratory systems. However, all these systems are deficient in principles, methodology, and methods of extrapolating the results of laboratory and semi-laboratory experiments to natural ecosystems. A mathematical theory of scaling of aquatic ecosystems could provide a scientific basis for developing the principles of such extrapolation. Scaling theory has proved to be useful in hydrodynamics and aerodynamics.

Let us recall the theory of dimensionality and scaling [3,4]. The main result is contained in the “S-theorem” (short for “similarity theorem”). We suppose that physical value a depends on determining parameters and variables $a_1, \dots, a_k$, $a_{k+1}, \dots, a_n$:

$$a = f\left(a_{1,\dots,}\ a_{k+1}, a_n\right). \tag{1}$$

If $a_1,\dots,a_k$ are independent variables then Equation (1) can be reduced to the relationship of dimensionless quantities:

$$S = F(1, \dots, 1, S_{k+1}, \dots, S_n),$$

where $S = a/a_1^h, \dots a_k^q; S_j = a_j/\left(a_1^{p_1^j}, \dots a_k^{p_k^j}\right); j = k+1, \dots, n,$ or compactly:

$$S = F(S_1, \dots, S_{n-k}). \tag{2}$$

It follows from (2) that S really depends—not on n parameters—but rather on $n - k$ parameters.

Let us apply the S-theorem to the simplest model of an aquatic microbial ecosystem based on the principle of a chemostat. Let a population of microorganisms of biomass $x(t)$ develop in the system at specific flow rate D (the ratio of volume flux to system volume) and consume some substrate of the background concentration $S(t)$ and the input concentration S_0. An increase in biomass of 1 gram requires the consumption of y grams of substrate. The dependence of the specific growth rate (SGR) of biomass (g) is given as $g = \mu S/(K_S + S)$, where μ is the maximum SGR, and K_S is the half-saturation constant for the substrate. Then

$$\left.\begin{aligned} S &= \varphi(x(0), S(0), S_0, t, \mu, K_s, D, y) \\ x &= f(x(0), S(0), S_0, t, \mu, K_s, D, y), \end{aligned}\right\} \tag{3}$$

where dimensionalities are as follows:

$$[x] = [S] = [x(0)] = [S(0)] = [S_0] = [K_S] = \mathrm{M/L^3};$$
$$[t] = T;\ [D] = [\mu] = T^{-1};\ [y] = 1.$$

As independent variables we take K_S and μ. Then, according to Equation (2), the dimensionless parameters are $F = x/K_S$, $W = S/K_S$, $\tau = t/\mu^{-1}$, $V = D/\mu$, etc. Equations (3) will be given as $W = \varphi(x(0)/K_S, S(0)/K_S, S_0/Ks, t\mu^{-1}, D/\mu, y)$ or $W = \varphi(\tau, V, y)$. Similarly, $F = f(\tau, V, y)$.

In contrast to an empirical search for Equation (2) type relationships, for this system there is a known mechanism, and thus dimensionless equations $W_\tau^* = (S_0/K_S - W)V - yWF/(1 + W)$ and $F_\tau^* = (W/(1 + W) - V)F$ can be written down. In the steady state $W = V/(1-V)$. A graph of a theoretical dimensionless relationship between the residual concentration of limiting substrate W $(= S/K_S)$ and the dimensional quantity of flow rate $V(=D/\mu;\ D<\mu)$ together with respective experimental values is presented in Figure 1. All undimensioned points are adequate (i.e., belong to) one and the same curve $W = V/(1 - V)$. Even this very simple example shows that the condition of similarity between field (f) and laboratory (l) ecosystems (i.e., equality of all dimensionless similarity parameters, $\tau_f = \tau_l$; $V_f = V_l$, etc.) leads to the requirement of a certain relationship between population microbiological parameter (μ) and flow rate (D) as a hydrodynamic quantity: $D_f/\mu_f = D_l/\mu_l$. Hence, in laboratory experiments, populations growing at higher rates μ_l can be used, and thus higher flow rates D_l can be set. The dimensionless laboratory relationship between the background concentration of the limiting substrate and D/μ will be the same as the field concentration. Since $t_f\mu_f = t_l\mu_l$, laboratory time (t_l) of the identical laboratory and field dynamics of the components will be μ_l/μ_f times shorter than the field time.

Using the S-theorem, one can write down simultaneous ecological–hydrophysical equations for the dynamics of the state of an aquatic ecosystem in dimensionless form. Thus, new parameters of similarity can be added to well-known ones (i.e.,Reynolds‘, Froude‘s, etc.), with ecological micro-parameters used along with hydrophysical ones. The future

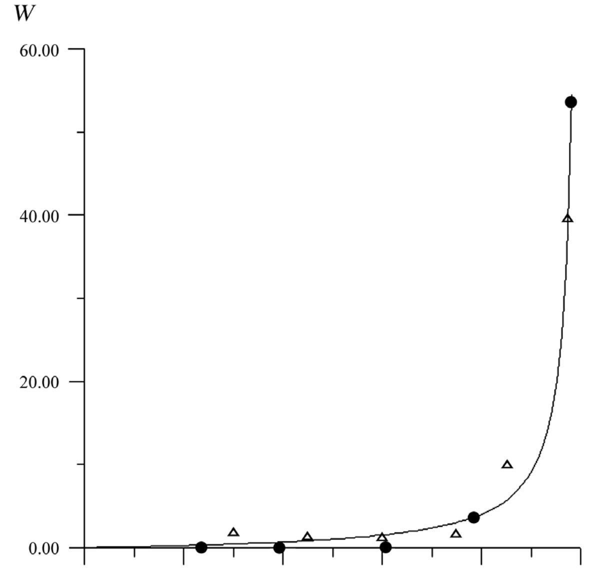

Figure 1. Dimensionless relationship between residual substrate concentration (N) and dimensionless flow rate (V). Experiments: *Saccharomyces carlsbergensis*, substrate, glucose [5]; Δ mixed culture of activated sludge, substrate, glucose [6]. Theory: —— $W = V/(1–V)$

scaling theory for aquatic ecosystems will contain a simultaneous mathematical description of the three main groups of processes: hydrodynamic, hydrochemical, and hydrobiological. The ultimate goal must be scaling of the maximally complete system of equations generally consisting of (1) a hydrodynamic unit, (2) a hydrophysical unit, and (3) an ecosystem unit. The objective of the hydrodynamic unit is to calculate the spatio-temporal dynamics of current velocity (depending on the morphometry of the water body floor, friction, slopes, water flow, and inflow). The objective of the hydrophysical unit is to calculate the dynamics of the following parameters: water temperature (depending on turbulence, heat balance with the atmosphere, and input of thermal effluents); the level of underwater irradiation (depending on the outer light flux, light absorption and reflection by microalgae and particles); sedimentation; turbidity; etc. The objective of the ecosystem unit is to calculate the dynamics of the concentrations of phytoplankton, zooplankton, bacteria, the main hydrochemical components, and pollutants in the water column, and the dynamics of bottom-water organisms (depending on biological interactions between populations, material cycling, industrial effluents, limiting factors, hydrophysical and hydrodynamic conditions, and sludge transport). The author is planning to create a computer system that will simulate these units, in dimensional and dimensionless forms, and inverse algorithms, which will reconstruct field dynamics from laboratory dynamics.

Having undimensioned macro-parameters of the system of the abovementioned groups of equations, we can make a universal undimensioned description of the dynamics of some ecosystems. Then, varying experimental dimensional microparameters, we may be able to find the values of undimensioned macro-parameters equal to real ones and conduct experiments with this small ecosystem. Conversely, experimental dynamics must be converted into real dynamics for a large ecosystem, which cannot be experimented on. Accurate similarity scaling can start a new direction in the experimental modeling of very many ecologically significant phenomena (material cycling in aquatic ecosystems, self-purification, stratification of biological components, migration of plankton, microalgal blooms) together with the modeling of hydrophysical parameters (currents, light and temperature fields, etc.). It would be good to use experimental facilities that hydraulic engineers have used for similarity scaling of hydrophysical characteristics only. For the sake of similarity, it will be necessary to equip these facilities with technical systems of light radiation for microalgal photosynthesis, to prepare model effluents, etc. The great advantage of this approach is that decision-makers would clearly see the environmental consequences of a given project even before it is practically implemented. First, it would be reasonable to construct simple homogeneous ecological flow-through systems and then gradually to move up to spatially heterogeneous ones. At the same time, it would be necessary to develop an ecological‒hydrophysical scaling theory, later involving the scaling of hydrochemical processes. In the course of development, theoretically grounded bans may be placed on simultaneous scaling of ecological‒hydrophysical processes that produce an opposite effect on scaling parameters, as happens in hydrodynamics in the case of wave resistance to movement $(Fr = \upsilon/\sqrt{lg})$ and in the case of viscose resistance $(Re = p\upsilon l/\mu)$. The main concerns of the scaling theory for aquatic ecosystems are (a) the validity of systems of equations and (b) the theoretical limits of similarity scaling.

3. GROWTH ACCELERATION: A NEW INTEGRAL INDEX OF THE CUMULATIVE EFFECT OF ALL THE REGULATORS IN A MONOCULTURE.

As the question of the complexity of ecosystems (Section 1.2) is rather difficult, the question of the non-trophic regulation of ecosystems should be pursued simultaneously. To create a stock of valid models, taking into account the mechanisms of population regulation (see Section 1.3), it is necessary to amass experimental data on the kinetic parameters of aquatic organisms, with kinetics being defined broadly (growth rates, food spectra, types of limiting factors, death rates, nature and intensity of inter-population relationships, etc.). These kinetics must be used in models along with quantitative field observations of the dynamics of ecosystem components so as to verify and identify the structures of model ecosystems. That is why the modeler‘s work cannot be independent of the experimenter‘s and the naturalist‘s work. They have to design experiments together.

Experimental methods must play a special part in the development of mathematical models of natural aquatic ecosystems, and specifically of microbial aquatic communities. The most important biochemical substances are those that are responsible for the sustainability of a microbial community. First of all, these are density-dependent growth control factors (DDGCFs; i.e., substances that are released or consumed by a population and that influence the growth of this or another population [7]). It is traditional to determine the relationship of the SGR to a specific DDGCF (e.g., a Monod-type relationship). However, the question of whether one such relationship is enough is not usually discussed (i.e., whether Liebig‘s bottleneck principle is valid here or the SGR depends on other DDGCFs, unknown to the researcher). In more general terms, this question can be formulated as follows. If we know the relationship of the SGR to some specific DDGCF, can we accurately quantify our knowledge of the density-dependent control of this species in a specific system? In other words, is there a way to determine the aggregate effect of all the DDGCFs on a specific population? In contrast to physics, where the types and number of forces and principles of their action are well-known, the situation in aquatic ecology is quite different. Any product of the ecosystem‘s metabolism (innumerable biochemical substances) can potentially be a factor controlling the stability of the community by positive or negative feedback. Even if we manage to make a complete list of all the biochemical products of metabolism, the main question remains open as to which of these substances can influence, say, the growth rate of a microbial population and how? Only these substances can be regarded as DDGCFs, which are essential for modeling.

The fundamental solution to this problem is based on an essentially physical idea. The idea is as follows. Take a separate microbial population, a monoculture, and assume that it is related to several biochemical DDGCFs by feedbacks. Microbiologists know that not only limiting substrates—but also metabolites—inhibiting or stimulating growth, can be considered to be DDGCFs. Then, what is the overall measure of the feedback level in growth control; that is, what is the estimate of the total effect produced by all the DDGCFs on population growth? As the theory developed previously states [8], this is a change in the growth rate increase B (i.e., acceleration of growth). Or, in other words, it is the rate of change of SGR, g, in response to a pulse disturbance of population concentration ΔX, under an unchanged (at the moment of disturbance) chemical composition of the environment:

$$B = \frac{\partial g}{\partial t}\Big|^{d} - \frac{\partial g}{\partial t}\Big|^{u} \quad (4)$$

where d is the disturbed state; u is the undisturbed state (the control state); and $[B] = T^{-2}$ (i.e. the dimensionality of growth acceleration value (B) is inverse to negative quadratic time $T(T^{-2})$; there is a similar value with similar dimensionality in Newton's mechanics called "physical object acceleration").

In the general case, for a monoculture whose SGR is determined by several (n) DDGCFs, the formula for calculation of the theoretical specific values of $B(B_{Th})$ is given as:

$$B_{Th} = \sum_{i=1}^{n} (\partial g / \partial A_i) a_i \quad (5)$$

where $g(A_1, A_2, ..., A_n)$ is the SGR of the monoculture as a function of all DDGCFs; and a_i is the coefficient of transformation of the i-th DDGCF.

Thus, all the n DDGCFs make a plus or minus contribution ($a_i \partial g / \partial A_i$) to the total theoretical value of B_{Th}. On the other hand, the same value can be found experimentally, B_E, from a change in the growth rate increase of a disturbed population and an undisturbed one, based on the above definition of feedback and Equation (4). It is assumed that growth rate increase as a response to the disturbance by biomass concentration occurs without any delay, due to the density activity of microorganisms (Figure 2). The value of $B_E - B_{Th} \equiv \Delta B$ determines the total control by unknown DDGCFs.

The proportion of total unknown DDGCFs in the total control (B_E) (i.e., $\Delta B/B_E$) can be determined, too. This is a very important value, showing the magnitude of the total control efficiency contributed by the yet unknown DDGCFs. If this value amounts to several dozen percent, a search for other DDGCFs should be continued. Strict equality of the positive feedback component to the negative one, so that $\Delta B = 0$, seems unlikely. As long as this variant has not been found in reality, we will not take it into account. In principle, the proposed method can be realized experimentally [8]. Based on this, we can estimate the contribution of specific regulators to the integral value of feedback and the natural (seasonal) values of feedback for natural populations of aquatic microorganisms in their natural habitats. Put in simpler terms, the experimental value of the natural negative feedback shows the degree to which the growth of a population of microorganisms is limited by natural substrates in a given place at a given time. A similar value obtained as a coefficient of interactions between populations shows the degree of competition or other types of relations.

Thus, in modeling the internal structure of a microbial community, the freedom of the model should be restricted by the requirement that the calculation should be in agreement with both classical kinetic parameters (production, generation time, the first-time derivatives of biomass) and new ones, values of natural feedbacks, and interaction coefficients (the second derivatives). A limitation "from above" is the requirement that the model should correspond to field monitoring data (e.g., biomass of species, or concentration of chemical substances such as zero derivatives).

4. CONCLUSION: THE FUTURE MONITORING OF AQYATIC ECOSYSTEMS.

We have proposed approaches to the study of ecosystems under natural and human-imposed conditions. These

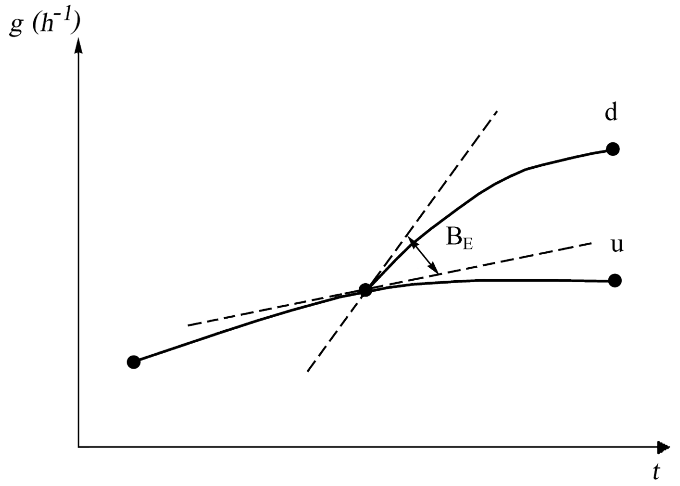

Figure 2. Approach to estimating the experimental level of feedback B_E

include (1) studying the fundamentals of the ecosystem similarity theory based on the principle of scaling however complex a system of equations may be necessary and getting a new set of dimensionless macroparameters and working out experimental approaches including the method of transfer of laboratory data to field data, (2) a new experimental–theoretical approach using the growth acceleration index to estimatef the integral degree of knowledge of growth regulators, (3) the idea of working out a new language to describe the state and dynamics of ecosystems with the help of specially selected bioassay indicators, and (4) based on the simple schemes of fermentation reactions, an idea is being developed about the possible dependence of a series of selective population parameters, which is important for modeling the microevolutional process. The proposed new trends of biophysical ecology will increase the physical strictness of the method.

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