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Entropy Index: New Opportunities in Assessing the Ecological State of Aquatic Ecosystems

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Abstract—The paper proposes a new method for the integrated assessment of aquatic ecosystems based on dissolved oxygen concentration and water body temperature. The study proves the validity of assessing the state of aquatic ecosystems in terms of entropy change and the possibility of assessing the ecological state of water bodies based on the point values of the entropy index. The algorithm for the calculation of the entropy index based on water temperature and oxygen concentration according to point measurements is described, and the theoretically reasoned scale for the estimation of the state of water ecosystems is proposed. Based on long-term data on dissolved oxygen and water temperature obtained at the stations of the state observation network and Roshydromet automatic water quality control stations, as well as on experimental data, the entropy index is calculated for some water bodies in the Russian Federation. The advantages and prospects of practical application of the method for the surface water monitoring are discussed.

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Keywords: Ecological state of a water body, dissolved oxygen concentration, water temperature, entropy index, aquatic ecosystems

INTRODUCTION

The problem of determination of the quality of water in water bodies based on the set of its physical and chemical properties, including the concentration of pollutants, is successfully solved in the system for monitoring the state and pollution of natural water implemented by Roshydromet. Hydrochemical observations at 2485 gaging stations cover 1180 water bodies. The determination of the ecological state based on assessing the state of living components of water bodies formed under given physical and chemical conditions is carried out at 274 gaging stations on 121 water bodies. Such insignificant level of observations is caused by the fact that the assessment of the ecological state of aquatic ecosystems is based on traditional hydrobiological approaches, that require significant labor costs and the availability of specialized and highly qualified staff. In addition, there is a methodological problem of assessing the ecological state. Namely, archaic methods based on saprobity, biotic, and other indices are used, not to mention the fact that the assessment of individual biotic communities is not identical to the assessment of the state of the ecosystem as a whole.

The solution to the problem of integrated ecological assessment of the water body state is, in the author’s opinion, in the area of thermodynamics, with its macroscopic approaches to the description of complex self-organizing systems.

DATA AND METHODS

Theoretical approaches to the assessment of the state of aquatic ecosystems based on thermodynamic parameters have been developed and verified in numerous experiments [3–5, 7]. A change in the entropy of an aquatic ecosystem caused by the photosynthetic production and destruction of organic matter is proposed as a criterion of the generalized ecological state of a water body; it is possible to calculate this parameter using the concentration of dissolved oxygen and water temperature [6]:

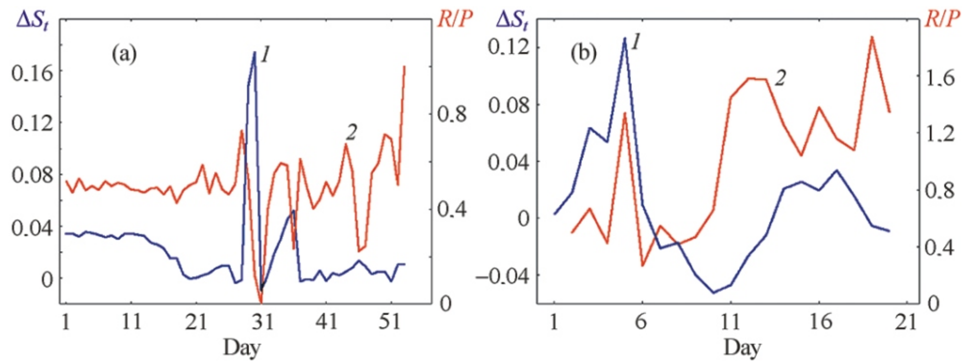

Fig. 1. The change in (*1*) entropy S_t and (*2*) balance ratio *R*/*P* (a) in the Zhizdra River and (b) in the model water ecosystem (mesocosm) under influence of cadmium sulfate.

$$S_t \quad \ln\frac{T_2}{T_1} \tag{1}$$

where $S_t = S_2 - S_1$ is the entropy change (the lower index t in S_t means that the time t = const, i.e., the entropy change depending rather on temperature than on time is considered); T_1 is water temperature in a water body; T_2 is water temperature corresponding to the 100% saturation with oxygen at the measured concentration. The entropy change calculated using (1) is a characteristic of production and destruction processes at a given time point and represents a derivative of entropy with respect to temperature. After that, similarly to the production-destruction parameters, it is possible to compute the time derivative for the entropy change in the daylight and in the dark [6]; it is also possible to use the ratio of the obtained values for assessing the aquatic ecosystem state based on the known criteria of the balance ratio [1].

Unfortunately, the proposed method cannot be widely implemented to the monitoring practice at the Roshydromet state observing network. The limitations are associated with a need in obtaining data on minimum and maximum daily oxygen concentration and water temperature, i.e., at least twice a day. This can be implemented only at automatic stations, the number of which at the Roshydromet network is limited.

At the same time, the value of the entropy change at a given time point can be presented as a result of the previous intra-reservoir processes, and, thus, it is possible to consider the point values of the entropy change as an adequate resulting estimate of the ecological state of the water body at a given place, that was formed during the preceding period. This is confirmed by parallel calculations based on data on the daily dynamics of water temperature and oxygen concentration obtained using the mobile automatic station of water quality control (ASKV-P, Taifun Research and Production Association) on the Zhizdra River.

Figure 1a presents the entropy change S_t computed from point measurements of oxygen concentration and water temperature in the morning under the minimum oxygen values, as well as the change in the dynamics of the balance ratio *R*/*P* (*R* is the destruction of organic matter in the dark, *P* is the primary production in the daylight) calculated from the daily oxygen concentration variation. It should be stressed that the entropy change is calculated using minimum daily oxygen values as they most adequately indicate a result of the interaction of two opposite processes of photosynthetic production and destruction of organic matter within a diurnal cycle. As clear from the figure, the graphs of *R*/*P* and S_t exhibit similar trends, and the entropy change S_t lags behind the change in the balance ratio *R*/*P* by 2–3 days. This corroborates a validity of the point estimation as a resultant of the preceding period and allows assessing the ecological state of water bodies based on the Roshydromet observations of oxygen concentration and water temperature.

The similar results were obtained from the comparison of the dynamics of *R*/*P* and S_t in mesocosms, in the experiments on studying the impact of cadmium on the model water ecosystems (Fig. 1b) [4].

Thus, the traditional hydrochemical parameters gain a deeper thermodynamic sense: they characterize a deviation of entropy of the aquatic ecosystem from the certain normal, whose degree determines a level of its wellbeing.

The previously published papers have repeatedly emphasized the value of thermodynamic approach for assessing the ecological state of water bodies, that allows giving a macroscopic description of their state in uniform terms and comparable values regardless of regional features and typology [3–5, 7]. For further development of this approach using the traditional hydrochemical parameters (dissolved oxygen concentra-

Table 1. The classification of the ecological state of water bodies

Water quality class	Entropy index	Ecological state
1	–0.123…0.062	Extremely favorable
2	0.063–0.124	Favorable
3	0.125–0.187	Satisfactory
4	0.188–0.249	Unfavorable
5	0.250–0.312	Extremely unfavorable

tion and water temperature) to calculate the entropy change and for the formalization of the estimates, it is necessary to form a theoretically reasoned scale of the state assessment.

As follows from formula (1), to calculate the value of S_t, the value of T_2 (water temperature corresponding to the 100% saturation with oxygen at the measured concentration) is determined using the oxygen solubility table. For example, the oxygen concentration measured in the water body was equal to 8.91 mg/dm^3, which corresponds to saturation concentration (equilibrium concentration) at the temperature of 21.0 C or 294.15 K. For the sake of brevity, let us call it "equilibrium" temperature. Water temperature measured in the water body was equal to 15 C or 288.15 K. The entropy change $S_t = \ln(T_2/T_1) = 0.021$.

The limiting values of the entropy change S_t in the water body can be computed proceeding from the extreme theoretically possible combinations of the values of oxygen concentration and temperature measured in the water body.

Let us assume that if water temperature in a water body T_1 = 273.15 K (0.0 C), the measured oxygen concentration C = 0.0 mg/dm^3. According to the oxygen solubility table, this corresponds to the equilibrium temperature T_2 = 373.15 K (100 C). In this case, the entropy change is maximal:

$$S_t \quad \ln\frac{T_2}{T_1} \quad \ln\frac{373.15}{273.15} \quad 0.312 \quad \max. \tag{2}$$

Such deviation of entropy implies almost the complete absence of photosynthesis, and the invasion is completely leveled by the oxygen consumption for the oxidation of organic and inorganic compounds. With the known assumptions, such state can be interpreted as an ecosystem death and is actually found in some water bodies subjected to extreme pollution.

If water temperature T_1 = 373.15 K (100 C), the measured oxygen concentration C = 14.62 mg/dm^3, which, according to the oxygen solubility table, corresponds to the equilibrium temperature T_2 = 273.15 K (0.0 C). In this case, the entropy change takes a theoretically minimal value:

$$S_t \quad \ln\frac{T_2}{T_1} \quad \ln\frac{273.15}{373.15} \quad 0.312 \quad \min.$$

However, the ecosystem life cannot exist at water temperature of 100 C (with an extremely rare exception of geothermal sources, where individual populations may exist, but there are no ecosystems). The maximum water temperature in the World Ocean is about 36 C [2], this value should be taken as an extreme, at which the ecosystem life is possible. This means that if water temperature T_1 = 309.15 K (36 C), the measured oxygen concentration C = 14.62 mg/dm^3, which, according to the oxygen solubility table, corresponds to the equilibrium temperature T_2 = 273.15 K (0.0 C). In this case, the entropy change takes a minimal value:

$$S_t \quad \ln\frac{T_2}{T_1} \quad \ln\frac{273.15}{333.15} \quad 0.123 \quad \min. \tag{3}$$

The mentioned range from 0.312 to –0.123 is divided into five classes corresponding to one or another state (see Table 1). The number of classes corresponds to the number of intervals used to classify a degree of water pollution accepted in Roshydromet. The negative values of S_t correspond to the oversaturated oxygen solution, whose existence is limited in time; it is extremely rarely found in the real water bodies and is unlikely in the morning, when the oxygen concentration in water is measured according to the method. Therefore, the negative values of entropy were included to the first class corresponding to the most favorable ecosystem state. For the sake of brevity, hereinafter the value of the entropy change S_t is called the entropy index.

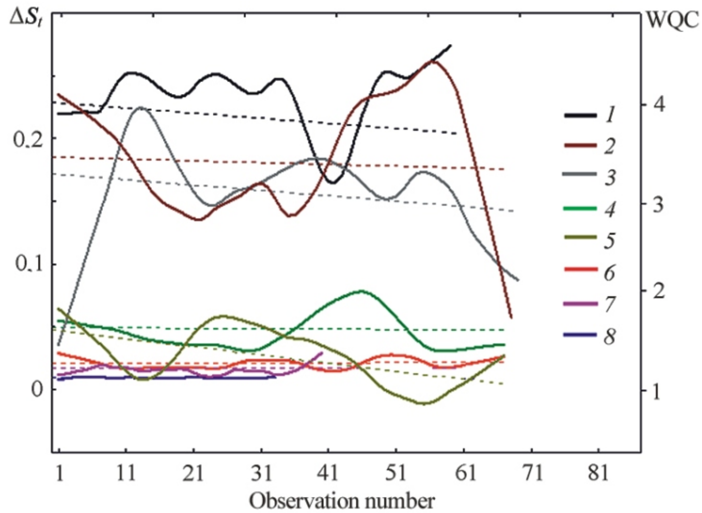

Fig. 2. The entropy index of water bodies S_t (the robust regression is the curves, the linear trends are the straight dotted lines of corresponding color) in comparison with the water quality class (WQC) based on the specific combinatory index of water pollution. (*1*) The Dachnaya River; (*2*) the Pel'shma River; (*3*) the Okhinka River; (*4*) the Nyuduai River; (*5*) the Pregolya River; (*6*) the Vite River; (*7*) the Lena River; (*8*) Lake Baikal.

RESULTS AND DISCUSSION

The estimate of the ecosystem state using the entropy index based on the proposed scale that indicates the ecosystem wellbeing, cannot always coincide with the pollution level estimate. This is explainable and does not contradict the meaning of the estimates. The degree of pollution characterizes the environmental quality, and the deviation of entropy from the normal characterizes the state of the ecosystem that exists in the given environment, i.e., the result of the pollution impact. The state of the ecosystem, the level of its wellbeing should not be directly linked to the degree of pollution of a water body for some reasons. One of the reasons is the possibility of the ecosystem adaptation to negative impacts, and the other is possible transformations of pollutants in natural water, that lead to changes in their toxic properties. However, it is obvious that an increase in the concentration of pollutants in water up to the critical level or their long-term impact can exceed the adaptation potential of ecosystems, which will lead to the change in their state.

The inconsistency of equating the level of pollution and the ecological state of a water body is well revealed during the field experiments with controlled introduction of pollutants. Figure 1b presents the graphs of variations in R/P and S_t in the mesocosm, where cadmium sulfate was introduced once at the beginning of the experiment, its concentration being 100 times higher than the maximum permissible one. Let us skip the detailed discussion of the response of the model ecosystem to the toxic impact and note that its state is within favorable. Similar results were obtained in numerous experiments in mesocosms using different toxicants with different concentration values and impact variants [5, 8].

To illustrate the application of the above classifier (Table 1), the assessment of the ecological state for a number of water bodies using the entropy index was carried out in comparison with the water quality class based on the specific combinatory index (Fig. 2). For clarity, knowingly clean water bodies (in particular, Lake Baikal, that is a priori considered as a reference water body) and objects with an extremely high level of pollution were selected. Long-term data on the oxygen concentration and water temperature obtained from the state observing network were used for calculations.

The estimates of the ecological state of the presented water bodies insignificantly differ from the pollution level estimates but basically correspond to the water quality class. The levels of pollution of the Dachnaya, Pel'shma, Okhinka, and Nyuduai rivers are estimated by the values of specific combinatory index within 5.5–8.3, which corresponds to the 4th–5th water quality classes. The graphs of entropy indices for these rivers characterizing their ecological state as unfavorable and extremely unfavorable are situated in the same region. The entropy indices of pure water bodies characterize their ecological state as extremely favorable and favorable. The most favorable state is registered for the Lake Baikal ecosystem. Attention should be paid to the pattern of the entropy index dynamics for water bodies with different levels of pollution. Pure, more favorable water bodies are characterized by more stable values of the entropy index. This regularity is important for assessing the state of water bodies. It indicates that ecosystems which are not subject to anthropogenic load and are in their natural state, provide balanced energy consumption in the stationary mode. It should be stressed that, in this context, the stability does not mean the resistance of ecosystems to external impacts. These peculiarities can indicate an unnatural state of aquatic ecosystems in polluted water bodies that regularly respond to negative external impacts.

CONCLUSIONS

The proposed approach based on the entropy index allows using traditional hydrochemical parameters (data on the concentration of dissolved oxygen and water temperature) to solve the problem of integrated assessment of the ecological state of water bodies. The advantages of such approach are evident. The base for the entropy index calculation is regular data obtained at the stations of all categories of the state observation network. The technique for the determination of oxygen concentration in water is simple and reliable, and the possibility of using the instruments (oximeters) significantly simplifies measurements and does not require highly qualified staff. The implementation of measurements in an automated mode with the transmission of data via wireless communication channels allows obtaining information about the state of water bodies in real time and, if needed, making timely management decisions.

The presented method for assessing the ecological state of water bodies can be a base for optimizing the system for the monitoring of the state and pollution of surface inland water. The assessment of the thermodynamic state of aquatic ecosystems in specific physical and chemical conditions allows evaluating an integrated impact of pollutants. The entropy index can be a final estimate of the ecological state of the water body classified as favorable; if the water body is classified as unfavorable, the index can be a base for making decisions on more detailed investigation. Such differentiated approach to the assessment of the ecological state allows reducing the number of pollutant observations in favorable water bodies and providing the detailed investigation of unfavorable ones.

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