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Exergy and ecological modelling of lake environment

Zhang Yong-ze

Environmental Engineering Center, Chinese Research Academy of Environmental Sciences, Beijing 100012, China

Wang Xuan

Institute of Environmental Science, Beijing Normal University, Beijing 100875, China

Abstract—The thermodynamic theories and ecological theories can be integrated effectively by exergy (biogeochemical energy of the system) to study the environmental problems of the lakes and reservoirs. In this paper, the applications of exergy in the ecological modelling of lake environment were reviewed. Results showed that exergy can be used as a goal function to estimate the parameters of the ecological model for lakes and reservoirs and to develop the structural dynamic models accounting for the changes in lake ecosystems, and as an ecological indicators for the development and evolution of lake ecosystems.

Keywords: exergy; ecological indicator; structural dynamic model; goal function.

1 Introduction

Increasingly serious lake eutrophication has become a global environmental problem and drawn great attention. In China, many lakes such as Lake Dianchi, Lake Chaohu, Lake Taihu *etc*. have been contaminated seriously, and their normal functions of supplying water, tourism, navigation and so on, have been affected by the serious lake eutrophication.

Lake ecosystem possesses immense complexities, which makes it impossible to analyze all the details of the system and therefore come to conclusions on ecosystem properties. In addition, because the system is more than the sum of its every part, the linkage between the biological and abiological components plays a major role and can only be accounted for by overviewing the entire system as a whole. Consequently, it seems of importance to attempt to capture ecosystem properties by using holistic methods and here thermodynamics seems to be an appropriate candidate (Jorgensen, 1992a).

The thermodynamic concept "exergy" is defined as the maximum amount of work a system can perform when it is brought to thermodynamic equilibrium with its environment. The environment could be defined as the inorganic soup on the earth 4 billion years ago before the biological evolution started(Jorgensen, 1977;1979). The maximum exergy principle and its use in relation to ecosystems was proposed in the late 70's(Jorgensen, 1979; Mejer, 1979) and has been established during the recent years.

In China, Zhou *et al*. (Zhou, 1997) have developed a new method for ecological energetics research-ecological exergy analysis, based on the exergy analysis in thermodynamics and the characteristics of living systems. In their study, the exergy balance equations for both an animal and a plant were constructed, and methods for estimating different types of exergy (chemical exergy, heat exergy, respiration exergy and photosynthetically active radiation exergy *etc*.) in living systems were proposed, then four ecological exergy efficiency indices for evaluating different ecological processes were proposed based on the exergy balance equations. In the study of lake eutrophication, exergy was used as an ecological indicator to describe the ecological changes of Lake Dianchi(Zhang, 1997a) and Lake Chaohu(Xu, 1997), and as a goal function to develop the structural dynamic model for Lake Dianchi (Zhang, 1997b).

In summary, because exergy has the following properties: a good theoretical basis in thermodynamics, close relation to information theory, clear and definite ecological meaning, rather high correlation with other goal functions and relative easiness of computation(Jorgensen, 1992b), it has been used widely as a goal function in ecological models to estimate the model parameters and develop the structural dynamic model accounting for the changes in lake ecosystem (Jorgensen, 1982; 1988; 1992a; 1992b; 1992c; 1994; Zhang, 1997b), and as an ecological indicator for the development state of the lake ecosystem(Salmonsen, 1992; Xu, 1997; Zhang, 1997a).

2 Exergy in ecosystems

The concept of exergy, through its definition by Evans (Evans, 1966) based on thermodynamic information, defined as deviation in entropy state of a system, finds its roots back in the classical thermodynamics and the earliest formulations of the second law by Carnot and Clausius. The entropy as a macroscopic property of a system was then defined as a function of microstates via the statistical thermodynamics founded by Boltzman and further developed by Gibbs. An important step since it is their formulations which makes it possible to calculate exergy (Nielsen, 1992).

Exergy, Ex, is defined by the following equation(Evans, 1969):

$$Ex = T_0(S_{eq} - S), \tag{1}$$

where, T_0, S are the temperature and entropy of the system respectively, S_{eq} is the entropy of the same system at thermodynamic equilibrium.

For an open system with inorganic net inflow and passive organic outflow, self-organization will affect the concentration of component chemical species and, therefore, the chemical contribution to exergy content. Assuming that temperature and pressure of the system(T and P) are the same than those of the environment (T_0 and P_0), exergy from Equation(1) becomes:

$$Ex = RT\sum_{i=0}^{n}\left[C_i \ln\frac{C_i}{C_{i,eq}} - (C_i - C_{i,eq})\right], \tag{2}$$

in which C_i and $C_{i,eq}$ are the concentration of the ith component in the far from equilibrium state and in thermodynamic equilibrium state respectively, C_0 is the concentration of the component in the inorganic matter, R the gas constant and T the absolute temperature(Mejer, 1979). By means of the above equation, Jorgensen(Jorgensen, 1995) derived a formula to evaluate the exergy of ecosystems:

$$Ex/RT = (\mu_1 - \mu_{1,eq})\sum_{i=1}^{N} C_i/RT - \sum_{i=2}^{N} C_i \ln P_{i,a}. \tag{3}$$

In Equation(3), μ_1 represents the chemical potential of detritus organic matter and $P_{i,a}$ is the probability to obtain a given component during the evolution by organizing organic matter according to information in genes. Aminoacids in living organisms are 20 and each gene determines a sequence of 700 aminoacids, thus:

$$P_{i,a} = 20^{-700r}.$$

$$(r = \text{number of genes in the organism}). \tag{4}$$

Therefore, the exergy can be calculated on the basis of existing studies on the evolution of DNA and genes in living organisms. Table 1 gives some average results for different organisms (Jorgensen, 1994).

Considering an aquatic environment, Equation(3) and Table 1 yield a simple formula to calculate the global exergy of the system:

$$Ex/RT = (1.79 \cdot 10^6) \cdot P + (104.9 \cdot 10^6) \cdot Z + (2.52 \cdot 10^8) \cdot F + (7.34 \cdot 10^5) \cdot (D + P + Z + F)(g/L), \quad (5)$$

in which, P, Z, F and D are the concentration (g/L) of phytoplankton, zooplankton, fishes and detritus organic matter, respectively. If the right hand of Equation (5) is divided by the detritus exergy coefficient (7.34×10^5), the same result expressed in grams of detritus equivalent can be obtained:

$$Ex/RT = (1)D + (3.4)P + (144)Z + (344)F \text{ (g detritus equivalent/L)}. \quad (6)$$

Table 1 Approximate number of genes in organisms and exergy conversion factors

Organism	DNA/cell, 10^{-12}g	Number of genes	Conversion factor
Detritus		0	1
Bacteria	0.005	600	2.7
Algae	0.009	850	3.4
Yeast	0.02	2000	5.8
Fungus	0.03	3000	9.5
Sponges	0.1	9000	26.7
Jellyfish/zooplankton	0.9	50000	143.9
Fish	20	120000	344
Field mouse	50	140000	402
Human	90	250000	716

Numbers in parentheses are conversion factors that give an approximate measure of the larger exergy contribution in P, Z and F, in comparison with detritus exergy D. Conversion factors account for the information embodied in the organism, in addition to the exergy of the biomass itself.

It can be concluded that the higher the exergy of the system, the higher the distance of the system from thermodynamic equilibrium as well as the contribution that can be obtained from it when appropriately used(Ulgiati, 1997), and different organizational levels could be measured by using their specific exergy content.

3 Applications of exergy in ecological modelling of lake environment

Exergy can be used as a goal function in ecological models to estimate the model parameters and develop the structural dynamic model accounting for the changes in lake ecosystem, and as an ecological indicator for the development state of the lake ecosystem. It has the following properties: (1) It is an energy term which is easily interpreted; (2) it is easily computed in the model; and (3) it is directly related to Darwin's theory and the application of exergy has therefore an ecological interpretation; and (4) it is dependent on the environment, and is not a state variable as entropy, which makes it better fitted to be used in ecology.

3.1 Estimating the model parameters

The parameter estimation is often "the weakest point" for many ecological models due to either (Jorgensen, 1992c) : (1) An insufficient number of observations to enable the modeler to calibrate the number of more or less unknown parameters; (2) no, or only a little information can be found in the literature; (3) ecological parameters are in general not known with sufficient accuracy; (4) the structure has dynamical behavior, i.e. the parameters are changing all the time, or (5) a combination of two or more of these points.

According to Darwin's theory, all the species in an ecosystem have the properties(i.e. the set of parameters) that are best fitted for survival under the prevailing conditions. The property of "survival" can be tested on the system level by use of exergy (Jorgensen, 1982; 1986; 1991), so the set of parameters that gives the best survivors can be found. Jorgensen (Jorgensen, 1992b) proposed a parameter combination modelling procedure based on the maximum exergy principle and Darwin's theory (Table 2).

Table 2 The parameter combination modeling procedure

Select parameters in accordance with species composition

↓

Select most crucial parameters

$P_1 = (P_{11}, P_{12}, \cdots\cdots, P_{1m})$

↓

Test after timestep t_p all combinations of

$$P_i = \begin{cases} P_{i1} - x\% \\ P_{i1} \\ P_{i1} + x\% \end{cases}$$

and select the combination that gives the highest exergy to be used as $P_2 = (P_{21}, P_{22}, \cdots\cdots P_{2m})$ for the timestep $t_p \to 2t_p$.

↓

⋮

↓

Test after timestep nt_p all combinations of

$$P_i = \begin{cases} P_{in} - x\% \\ P_{in} \\ P_{in} + x\% \end{cases}$$

and select the combination that gives the highest exergy to be used as $P_{n+1} = (P_{(n+1),1}, P_{(n+1),2} \cdots\cdots P_{(n+1),m})$ for the timestep $nt_p \to (n+1)t_p$

The above parameter combination modelling procedure was applied by Jorgensen (Jorgensen, 1992b) to study Sobygaard Lake and OECD-lakes. In the study of Sobygaard Lake, the maximum growth rate, settling rate and grazing rate of phytoplankton were selected as the most crucial parameters (Table 3). As can be seen, the proposed procedure is able to simulate approximately the observed changes in phytoplankton parameters. The growth rate is reduced by 40% from 2.0 day^{-1} to 1.2 day^{-1} which is approximately in accordance with the increase in size. It was observed that the phytoplankton average size was increased from 100 μm^3 to 500—1000 μm^3. The studied results of OECD-lakes had shown that the turnover rate coefficient (k_{TR}) values giving the maximum exergy were qualitatively in accordance with Vollenweider's (Vollenweider, 1975) results.

3.2 Developing the structure dynamic model for lakes and reservoirs

Table 3 Parameter combination giving the highest exergy

	Max. growth rate, day^{-1}	Settling rate, $m.day^{-1}$	Grazing rate, day^{-1}
1985	2.0	0.15	0.24
1988	1.2	0.45	0.132

The development of the structure dynamic models has recently been developed as a research direction within the traditional established discipline of ecological modelling (Jorgensen, 1986; Nielsen, 1992). The term structural dynamic refers to the ability of the models to perform changes in species composition and trophic structure of the ecosystem modeled. The development of this type of model was started in the area of aquatic ecosystem models, especially lake ecosystems, where the models through some years have reached a state to certain degree, they are able to give acceptable prognosis of the quantitative development of ecosystem as a consequence of changes in external factors influencing the system.

In general, the model constraints should include the conservation principles, the chemical composition and the law of thermodynamics, however, only a few models can include the ecological constraints due to under-consideration of the properties of ecosystem. Based on the above analyses, Darwin's theory "survival of the fittest" can be quantified by exergy as an ecological constraint to the ecological models.

The changes in lake ecosystem should be reflected by the changes in parameters in the model

(Zhang, 1995). However, in most studies, the main parameters (such as the maximum growth rate of phytoplankton *etc*.) are often taken as constants, which makes the ecological model ecologically less reasonable. Exergy can be used as a goal function, i.e. an ecological constraint in the ecological model, due to its above mentioned advantages. By application of exergy, the maximum exergy principle and Darwin's theory can be used to construct the above parameter combination modelling procedure, which allows a continuous development of the essential parameters of the model during simulation in accordance with the optimized function.

In the study of Lake Dianchi (Zhang, 1997b), exergy was introduced into ecological model as a goal function of the maximum growth rate, settling rate of phytoplankton, the maximum growth rate of zooplankton to develop a structural dynamic model for Lake Dianchi, and parameter combinations were carried out by using the above modelling procedure. In Lake Dianchi, phosphorus is the main limiting factor of nutrients, so only the contribution to exergy from the phosphorus cycle was considered. In the study, exergy was computed using Equation(2), the state variables included the concentrations of phosphorus in algal cells, soluble phosphorus, phosphorus in detritus and phosphorus in zooplankton. The results followed that this model can account for the changes in the ecological structure and species composition of lake ecosystem, and the changes in lake ecosystem can be reflected by the changing model parameters and the changing exergy values.

A structural dynamic model had been developed by Nielsen (Nielsen, 1992) in order to describe the shifts in composition of the phytoplankton society and tropic structures in a Danish shallow lake (Lake Vang) as response to change in loading or biomanipulation. In this model, phosphorus was taken as the only limiting nutrient; the development of the phytoplankton society was chosen to be governed by a combination of the following factors: growth processes, loss processes, higher tropic levels, biological compartment 9 (9 types of algae were included in the model: microcystis, aphanizomenon, stephanodiscus, asterionella, pediastrum, scenedesmus, dinobryon, peridinum and cryptomonas); the growth and the development of the phytoplankton society were governed by the grazing on phytoplankton and described as an ordinary Monod kinetic relationship and loss rate were included as an assimilation coefficient and excretion; the biological model was combined with a simple flow-ratio based hydrological model, chosen to be sufficient to simulate the hydrodynamics in this lake. The results indicated that exergy may play an important role in governing the development of the phytoplankton society.

Species composition often tells more about the condition of a lake or reservoir than water quality. The presence of blue-green algae or toxic algae is much greater environmental problem than a low transparency or a high nutrient concentration. In Jorgensen and Nielsen's (Jorgensen, 1994) study, a two-classes phytoplankton model (diatoms and green algae) had been developed to try to predict the shifts in species composition between the dry and the rainy seasons. In this model, two nutrients were considered: phosphorus and silica. The settling rate for the diatoms was set to 0.5m/day, but with a relation between the precipitation and the settling which will reduce the settling rate to 0.15m/day at the most rainy days. For green algae the settling rate was 0.2m/day in the dry season with a reduction to 0.1m/day in the rainy season. The results had shown that dominance of diatoms gave the highest exergy in the rainy season under the given circumstances (temperature, solar radiation, the stirring up effect of the rain and the retention time). Meanwhile, the distribution between the two classes of algae in the dry period gave the highest exergy.

In the study of Lake Glumso, exergy was used by Salomonsen and Jensen (Salomonsen, 1996) as a measure of build-up of biological structure. Data from lake Glumso for the period 1981—1984 were chosen for the study, in that period, the lake underwent a change in phytoplankton species composition. The study had shown that the two phytoplankton groups(chlorophytes and diatoms) did perform a larger build-up of exergy than if only one of the groups had been presented, and that the calibrated growth parameters for the chlorophytes represented the highest build-up of exergy while the results for the diatoms were less univocal.

All the above studies have followed that exergy can be used as a goal function to develop the structural dynamic models for lakes and reservoirs to describe the shifts in the species composition and the changes in ecological structure of ecosystem, and used widely in the ecological modelling of lake environment.

3.3 Indicating the development and evolution of lake ecosystem

After a few decades of research, there are several indicators that making thermodynamic approach to living organisms and biological systems and trying to interpret and understand them within a thermodynamic framework. Life does not violate nor does it disobey the second law of thermodynamics, but rather exists because of it. Exergy in that sense could turn out to be a basic concept for understanding complex structures such as ecosystems, since they can be interpreted within this concept, i.e. the behavior and evolution of ecosystems can be analyzed using exergy as indicator of quality and basis for selectional process(Nielsen, 1992). To be able to express or explain ecosystem behavior, exergy should also be meaningful to all or most of the terms normally used within the established ecosystems science, such as order, organization, complexity *etc*.

The thermodynamic approach to ecosystems is but one of several other theories that claim to be important in the studies of ecosystems in order to understand their enormous complexity and how they behave and evolve with time. Some of the concepts like "exergy" are proposed to be used as "goal functions", i.e. properties that direct ecosystem evolution. The proposed goal functions are as follows: ascendancy (Ulanowicz, 1986), biomass (Straskraba, 1983), maximum power (Odum, 1983), emergy(Odum, 1983), maximum entropy(Schneide, 1988), exergy (Jorgensen, 1982) and so on.

Jorgensen(Jorgensen, 1992a) introduced exergy as the holistic property of ecosystems and presented a tentative thermodynamic law ELT(the ecological law of thermodynamics). This law can be considered as a translation of Darwin's theory in thermodynamics and presented as: a system with a through-flow of exergy will attempt to utilize the flow to increase the exergy of the system, and the organization of the system that is able to give the system the highest exergy will be selected. This law indicated that ecosystem develop towards the highest possible exergy.

Bastianoni and Marchettini(Bastianoni, 1997) took the emergy/exergy ratio as a measure of the level of organization of systems. To test this approach three coastal lagoons were considered, two of them were artificial, built by man to purify sewage, the third system was the lagoon of Caprolace(Italy) a "natural" system. The experimental results showed that the emergy/exergy ratio had the lowest value for the ecosystem of Caprolace. The waste pond had the highest environmental cost for the production of a unit of organization. Both the control and the waste ponds showed a decreasing value of the emergy/exergy ratio with time, meaning that natural selection was organizing the systems.

Salomonsen(Salomonsen, 1992) examined the properties of exergy, power and ascendancy in a moderately productive lake and in a highly productive lake using two steady-state models. The results showed that the exergy of all the tropic compartments was higher in the eutrophic lake than in the oligotropic lake. This is an effect of the increased biomass.

Xu(Xu, 1997) took exergy and structural exergy as ecological indicators to describe and measure the development state of the Lake Chaohu ecosystem by demonstrating and analyzing their relationships to tropic state, biodiversity, biomass and species composition. The findings for Lake Chaohu ecosystem revealed that structural exergy had negative correlation to tropic state ($r = -0.66$) and positive correlation to biodiversity($r = 0.75$); however, exergy had a strong positive correlation with biomass($r = 0.94$). Therefore, it was concluded that exergy and structural exergy may serve as the ecological indicators to give appropriate information on the development state of the Lake Chaohu.

Ecosystem are too complex to be viewed in every detail. To keep track of their dynamics there is therefore a need for holistic approaches. The thermodynamic theories, such as the maximum exergy principle, can provide such approaches.

4 Conclusions

Exergy can be used as a goal function because it has the following advantages compared with other thermodynamic concepts: (1) It is an energy term which is easily interpreted; (2) exergy is easily computed in the model; (3) it is directly related to Darwin's theory and the application of exergy has therefore an ecological interpretation; and (4) it is dependent on the environment, and is not a state variable as entropy, which makes it better fitted to be used in ecology.

The applications of exergy in the ecological modelling of lake environment have shown that exergy can be used to estimate the model parameters and develop the structural dynamic model to account for the changes in species composition and ecological structure of the lake ecosystem, and indicate the development and evolution of the lake ecosystem. The thermodynamics provide a holistic approach for analyzing and understanding the lake ecosystems.

However, in order to use effectively exergy in the ecological modelling of lake environment, the following work should be carried out further:

Observing and collecting the enough data on the concentrations of nutrients, the biomasses of phytoplanktons, zooplantktons and fishes and so on, which can indicate comprehensively the state of lake eutrophication and the development state of lake ecosystems.

Taking the contribution of different nutrient cycles(such as phosphorus cycle, nitrogen cycle, carbon cycle and silica cycle *etc*.) to the exergy of lake ecosystem into account in the computation of exergy as much as possible.

Considering the changes in exergy of lake ecosystem caused by the change in the ecological structure of lake and the changes in the external forcing functions (such as meteorological conditions, pollutant loads *etc*.) respectively, so that the changes in lake ecosystem can be described well by the change in exergy.

Selecting the reasonable algorithm can perform the changes of the model parameters with time in the modelling processes, consequently, the changes in lake ecosystem can be reflected indirectly by the varying model parameters and the varying exergy.

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