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## Thermodynamics and ecology<sup>☆</sup>

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#### Abstract

How to apply thermodynamic methods and concepts to ecology, how to describe the ecosystem's behaviour in terms of physics (and particularly, thermodynamics), what kind of physical criteria can be used for estimation of anthropogenic impact on ecosystems? — I try to answer these questions in this manuscript. From the viewpoint of thermodynamics, any ecosystem is an open system far from thermodynamic equilibrium, in which entropy production is balanced by the outflow of entropy to the environment. I suggest the 'entropy pump' hypothesis: the climatic, hydrological, soil and other environmental conditions are organised in such a way that only a natural ecosystem which is specific for these conditions can be in the dynamic equilibrium (steady-state). In the framework of this hypothesis I can calculate the entropy production for the ecosystem under anthropogenic stress. This approach was applied to the analysis of crop production in Hungary in the 1980s. Considering systems far from thermodynamic equilibrium we can prove that the so-called exergy is a functional of a dissipative function, which is undertaken along the trajectory from a thermodynamic equilibrium to a dynamic one. It was shown there is a close connection between the measure of additional information (Kullback's measure) and exergy. © 2000 Elsevier Science B.V. All rights reserved.

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### 1. Introduction

Quoting from table-talks in Moscow:

Thermodynamics is full of highly scientific and charming terms and concepts, giving an impression of philosophical and scientific profundity. Entropy, thermal death of the Universe, ergodicity, statistical ensemble — all these words sound very impressive posed in any order. But, placed in the appropriate order, they can help us to find the solution of urgent practical problems. The problem is how to find this order... In 1948 John von Neumann said:

... nobody knows what entropy is in reality,

that is why in the debate you will always have an advantage

Many studies are known which attempt to apply (directly or indirectly) thermodynamic concepts and methods in theoretical and mathematical ecology for the macroscopic description of biological communities and ecosys-

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tems. Such attempts can be divided into two classes.

The first class includes the direct transfer of such fundamental concepts as entropy, the First and Second Laws of Thermodynamics, Prigogine's theorem, etc., into ecology. The literature on this subject is enormous: recent publications are Weber et al. (1988), Jørgensen (1992), Schneider and Kay (1994).

The second class includes some attempts to use the methods of thermodynamics, such as Gibbs statistical method. Khinchin (1943) has proposed a very elegant scheme for the construction of formal statistical mechanics. This scheme could be applied to a wide class of dynamical systems, in particular, to Volterra's 'prey-predator' system (Kerner, 1957, 1959; Alexeev, 1976). Unfortunately, none of these results can be interpreted satisfactorily from the ecological point of view (Svirezhev, 1976).

Strictly speaking, there are no principal prohibitions to applying thermodynamic concepts to such physical-chemical systems as ecological ones. The problem is the following: there is no direct homeomorphism between the models (in a broad sense) in thermodynamics and the models in ecology. For example, the model of ideal gas (the basic model of thermodynamics) cannot be applied directly to a population or, moreover, to a biological community. The macroscopic state of the ideal gas is an additive function of the microscopic states of molecules. The stable structure of a biological community is the consequence of interactions between populations rather than the function of characteristics of individual species, etc. It is appropriate to mention the well-known ecological paradox: the diversity of a community is maximal when the distribution of species is uniform, i.e., when there are no abundant and rare species, and no structure.

But in spite of this, I look at the problem of the application of thermodynamic ideas to ecology with optimism. I think that if we could manage to formulate the thermodynamic-ecological model correctly, and if we were able to formulate correctly the concept of the thermodynamic system in relation to ecosystems, the use of these formulations in ecology would be very fruitful.

# 2. The physical approach: direct calculation of the entropy and the 'entropy pump' hypothesis

From the viewpoint of thermodynamics, any ecosystem is an open thermodynamic system. The climax of the ecosystem corresponds to a dynamic equilibrium (steady-state), when the entropy production inside a system is balanced by the entropy flow from the system to its environment. This work is being done by the 'entropy pump'. What does mean this?

Let us consider one unit (hectare, m<sup>2</sup>, etc.) of the Earth's surface, which is occupied by a natural ecosystem (meadow, steppe, forest, etc.) maintained in a climax state. There is a natural periodicity in such a system (1 year); during this period the internal energy of the ecosystem is increased by a value of gross primary production (which can be expressed either in calories or in joules). One part of the production is used for respiration with further transformation into heat, while another part (the net primary production) turns into litter and other forms of soil organic matter and is taken by consumers. (The relatively small amount of latter is mainly spent in supporting the consumer's metabolism and finally it also transforms into heat. Therefore formally the latter may be included in plant respiration.) But, since the system is at dynamic equilibrium, an appropriate part of dead organic matter in litter and soil has to be decomposed (releasing a place for 'new' dead organic matter from annual net primary production). The 'old' dead organic matter has 'to be burned', so that its chemical energy is transformed into heat. The temperatures and pressures in the ecosystem and its environment are assumed to be equal, i.e., we consider some isothermal and isobaric process.

In the theory of open systems the total variation of entropy is presented in the form of two items:

$$dS(t) = d_i S(t) + d_e S(t), \qquad (1)$$

where  $d_i S(t) = dQ(t)/T(t)$ , dQ(t) is the heat production caused by irreversible processes within the system and T(t) is the current temperature (in K) at a given point of the Earth's surface. The value  $d_e S(t)$  corresponds to the entropy of exchange processes between the system and its environment. In fact, total heat production = heat emission of the plant metabolism (heat emitted during the process of respiration),  $R_v(t)$ , + heat emission of the consumer's metabolism,  $R_c(t)$ , + heat emission of the decomposition of 'dead' organic matter, D(t). Really  $R_v(t) > > R_c(t)$ , so that the total metabolism of the ecosystem is equal to the metabolism of its vegetation, in practice.

Integrating Eq. (1) in respect to 1-year natural period we get

$$S(t+1) - S(t) = \int_{t}^{t+1} \frac{R_{v}(\tau) + D(\tau)}{T(\tau)} d\tau - \delta_{e}S,$$
(2)

where

$$\delta_{\rm e} S = \int_t^{t+1} \frac{{\rm d}_{\rm e} S}{{\rm d}\tau} \, {\rm d}\tau \, .$$

Applying the mean value theorem to the integral in Eq. (2) we get

$$\int_{t}^{t+1} \frac{R_{v}(\tau)}{T(\tau)} d\tau = \frac{1}{T(\theta_{1}^{t})} \int_{t}^{t+1} R_{v}(\tau) d\tau = \frac{1}{T(\theta_{1}^{t})} [P_{0}(t) - P_{0}^{n}(t)], \ \theta_{1}^{t}, \ \theta_{2}^{t} \in [t, t+1],$$

$$\int_{t}^{t+1} \frac{D(\tau)}{T(\tau)} d\tau = \frac{1}{T(\theta_{2}^{t})} \int_{t}^{t+1} D(\tau) d\tau = \frac{1}{T(\theta_{2}^{t})} \widetilde{D}_{0}(t),$$

The values  $P_0(t)$  and  $P_0^n(t)$  are annual gross (total) and net primary productions, and the temperatures  $T(\theta_1^t)$ ,  $T(\theta_2^t)$  are some 'mean' annual temperatures (they may be different!). In all these values the notation 't' means a number of the corresponding year.

In spite of the fact that the state of the ecosystem changes within a 1-year interval, we can consider the climax natural ecosystem as a stationary system, if the time step is equal to 1 year. Therefore, since the system is in the dynamic equilibrium (steady-state) then the 'burned' part of the dead organic matter  $\tilde{D}_0(t) = P_0^n(t)$  and, moreover, in Eq. (2) S(t+1) - S(t) = 0. Then

$$\delta_{e}S(t) = \frac{1}{T(\theta_{1}^{t})} P_{0}(t) + \left[\frac{1}{T(\theta_{1}^{t})} - \frac{1}{T(\theta_{2}^{t})}\right] P_{0}^{n}(t).$$
(4)

Considering the integral

$$\int_{t}^{t+1} R_{v}(\tau) d\tau = \int_{t}^{t+1} r(\tau) p_{0}(\tau) d\tau$$
$$= r(\theta_{3}^{t}) \int_{t}^{t+1} p_{0}(\tau) d\tau$$

$$= r(t)P_0(t), \ \theta_3^t \in [t,t+1],$$

where  $r(\tau)$  and  $p_0(\tau)$  are the current respiration coefficient and total primary production within a 1-year interval, respectively, and  $r(\theta_3^t) = r(t)$  is a 'mean' respiration coefficient, so that  $P_0^n(t) = [1 - r(t)] P_0(t)$ , and we also get

$$\delta_{\rm e} S(t) = \left\{ \frac{1}{T(\theta_1^t)} \left[ \frac{2 - r(t)}{1 - r(t)} \right] - \frac{1}{T(\theta_2^t)} \right\} P_0^{\rm n}(t).$$
(4')

In accordance with our assumption, the entropy  $\delta_e S(t)$  must be 'sucked out' by the solar 'entropy pump' (a steady-state condition). Consequently, the power of this pump at some point of the Earth is equal to  $\delta_e S(t)$ .

Note that the process of the formation of a new biomass and its next degradation represents a complex chain of multiple chemical and biochemi-

(3)

cal reactions. In our approach, which is based on the Hess theorem (see, for instance, Rubin, 1967), we assume that the total entropy produced by this chain depends only on the thermodynamic characteristics of the initial and final elements, i.e. it is only determined by the chain input and output.

The entropy, which is produced by the destruction of chemical structure of biomass, is considerably less than the 'heat' entropy. Hence, we can neglect the structural entropy (for balance calculations).

We already mentioned above that in the general case  $T(\theta_1') \neq T(\theta_2')$ . However, if we take into account that both the photosynthesis and the respiration, and also the decomposition of dead organic matter, depend on the current temperature in a similar way then we can assume that  $T(\theta_1') \approx T(\theta_2') = T(t)$ . Apparently the best approximation for this 'mean' temperature will be the mean active temperature, i.e. the arithmetic mean of all temperatures above 5°C, which is a good indicator of biological activity. The next approximation may be the mean temperature of a

vegetation period. Finally the annual mean temperature is possibly not approximated very well.

If we accept this assumption then Eq. (4) and Eq. (4') are re-written in the form

$$\delta_{\rm e}S = \frac{P_0}{T} = \frac{1}{1-r} \frac{P_0^{\rm n}}{T}.$$
(5)

Let us assume that the considered area is influenced by anthropogenic pressure, i.e. a flow of artificial energy (W) into the system takes place. We include in this definition ('the flow of artificial energy') both the direct energy flows (fossil fuels, electricity, etc.) and the inflow of chemical elements (pollution, fertilisers, etc.). We suppose that this inflow is dissipated within the system and transformed into heat and, moreover, modifies the plant productivity.

Let the gross production of the ecosystem under anthropogenic pressure be  $P_1$  (in caloric units or joules). We assume that despite anthropogenic perturbations the ecosystem remains in a steadystate. Using the previous arguments we get

$$\delta_{e}^{1}S = \frac{1}{T}(W + P_{1}).$$
(6)

We make a very important assumption and suppose that a part of the entropy released at this point by the 'entropy pump' is equal, as before, to  $\delta_e S = P_0/T$ . Really, we assume that the power of the local entropy pump corresponds to a natural ecosystem, which would be situated in that location. In other words, climatic, hydrological, soil and other environmental local conditions are organised in such a way that only a natural ecosystem which is specific namely for this combination can be in a steady-state without environmental degradation.

This is the 'entropy pump' hypothesis.

If we accept it we must also assume that the transition from natural to anthropogenic ecosystem is performed sufficiently fast in order that the 'adjustment' of the entropy pump is not changed. Therefore, in order that another (uncompensated by the entropy pump) part of the entropy

$$\delta_{\rm e}^2 S = \sigma = \delta_{\rm e}^1 S - P_0/T \tag{7}$$

should be compensated by the outflow of entropy to the environment, only one way exists. This compensation can occur only at the expense of environmental degradation ( $\sigma > 0$ ), resulting, for instance, from heat and chemical pollution, and mechanical impact on the system. Substituting Eq. (6) into Eq. (7) we get

$$\sigma T = W + P_1 - P_0 \,. \tag{8}$$

The values in Eq. (8) are not independent. For instance,  $P_1$  depends on W. Since we are not able to estimate this correlation within a framework of theory of thermodynamics, we have to use empirical correlation. The second problem is how to define the reference state  $P_0$ , the productivity of what kind of natural ecosystem must be chosen. For this we consider one new concept.

We assume that the relation of succession connects the 'natural' and 'anthropogenic' ecosystems. In order to explain the new concept and a few accompanying definitions, which is very important for our thermodynamics approach, we consider the following 'Gedankenexperiment'.

Let us image that we have stopped all the anthropogenic energy and chemical fluxes into the ecosystem. As a result, succession from the anthropogenic ecosystem towards one of 'natural' ones is started. If the anthropogenic pressure has been weak and its impact has been relatively short, so that the environment was not seriously degraded, then the 'natural' ecosystem will be typical of a 'wild' ecosystem previously existing in this locality before the anthropogenic ecosystem. This would be forest, grassland, steppe, etc. This is a typical reversible situation. Under severe degradation succession would also take place, but towards a different type of ecosystem, for instance, a ruderal one. This is quite natural, since the environmental conditions have been strongly disturbed (for instance, as a result of soil degradation). This is an irreversible situation. Since we want to remain in a framework of 'reversible' thermodynamics we shall consider only the first case where the anthropogenic impact is relatively weak.

The time-scale of succession, i.e. a transient time from the anthropogenic ecosystem to natural one, depends on what kind of ecosystem is considered as a natural one. If the natural ecosystem is, for instance, a grassland then the transient time (several years) will be compared to the time-scale of our thermodynamic model (1 year), where the equilibrium entropy balance is calculated for 1 year. In this case  $P_0$  is the productivity of the corresponding grassland community.

The situation becomes more complex, if the final state of succession is a forest. Then the transient time will be approximately equal to 100 years and it is much greater than the model time-scale. Thus, there are two different time-scales, so that the equilibrium entropy balance is calculated in respect to a fast time (years), while the successional dynamics of productivity is considered in a slow time (100 years). In this case succession can be considered as a thermodynamically quasi-stationary process (simultaneously, we remain in the frameworks of equilibrium thermodynamics). Then the values  $P_0$  and  $P_1$  in Eq. (8) cannot significantly differ from each other. If we consider their ranking along the temporal axis of succession then  $P_0$  must be the productivity of such stage of the successional ecosystem, which is distant from the starting point by the model time-scale (several years). In other words, the next stage of the succession must be a 'natural' ecosystem in our sense. For instance, if the anthropogenic ecosystem is an agro-ecosystem, and a typical ecosystem for given location is a forest, then a grass-shrubs ecosystem (not a forest) will be our 'natural' ecosystem. And finally, we introduce a new definition: a successionally closed ecosystem is the first stage of succession of an 'anthropogenic' ecosystem when the anthropogenic pressure is removed.

What is a 'dynamic' sense of the 'successional closeness', and why do we need such a concept? The main restriction in our approach is the following: only close steady-states can be compared, and their vicinities in the model phase space must intersect significantly. And what is more, the times of fast transitions between these steady-states, from a natural to anthropogenic ecosystem and vice versa, must be small (in comparison with the time-scale of succession).

If we keep in mind the sense of  $\sigma$ -value, it is obvious that its value can be used as a criterion for environmental degradation or as an 'entropy fee', which has to be paid by our society (in fact, suffering from the degradation of environment) for modern industrial technologies. Certainly, there are other ways to compensate the entropy produced within the system. For instance, we can use additional inputs of artificial low-entropy energy, which will be spent for soil reclamation, pollution control, or, generally, for wide use of ecological technologies. Using the suggested method of entropy calculations the needed investments should be estimated in energy units.

### 3. Case study: the Hungarian agricultural system

If the annual total (gross) agro-ecosystem production is equal to  $P_1$ , the net production is equal to  $(1-r)P_1$  where r is the respiration coefficient, and the term  $rP_1$  then describes the respiration losses. The kth fraction of the net production is being extracted from the system with the yield, so that the crop yield is equal to

$$y = k(1 - r)P_1$$
. (9)

The remaining fraction  $(1-k)(1-r)P_1$  is transferred to the litter and soil. If we accept the stationary hypothesis then we must assume that the corresponding amount of litter and soil organic matter must be decomposed. Concerning the extracted fraction of production we assume that this fraction does not take part in the local entropy production. And finally, the entropy balance of this system will be (Eq. (8))

$$\sigma T = W + (1-k)(1-r)P_1$$
  

$$+ rP_1 - P_0$$
  
respiration - respiration -

where  $P_0$  is the gross production of a successionally closed ecosystem. (In our case this is commonly called 'old field succession'.)

Note that for the first ('robust') estimation we sum all the energy flows (fuels, machinery, etc.) and chemical flows (fertilisers and pesticides) into one (artificial energy) inflow W.

The problem is (and this was mentioned above) how to find the relation between  $P_1$  and W? Let us remember the eco-energetics analysis by Pimentel (1980). He suggested that the relation between the crop and the input of artificial energy is linear,  $y = \eta W$ . The empirical coefficients of energy efficiency,  $\eta$ , were calculated for different agro-ecosytems in many countries and various regions.

In fact, the coefficient  $\eta$  is a modification of the efficiency coefficient well-known in thermodynamics, which is a consequence of the First Law. In thermodynamics it is usually less than one, but in contrast, the coefficient  $\eta$  may be more than one. The point is that formally we must take into account the solar energy  $(E_s)$  and the correct form for the efficiency coefficient will be  $\eta' = y/(W + E_s)$ . In this case what does Pimentel's coefficient  $\eta$  mean? It is obvious that  $y = y(W, E_s)$ , and linearising y at W = 0 we get

$$y(W,E_{\rm s}) \approx y(0,E_{\rm s}) + \left(\frac{\partial y}{\partial W}\right)_0 W.$$
 (11)

Here we assume that the first term is negligibly small in comparison with the second one and the derivative  $(\partial y/\partial W)_0 = \eta = \text{const}$  for considered values W. Then we immediately get Pimentel's relation  $\eta = y/W$ . In fact, this reasoning is not rigorously correct, but it allows us to use a lot of empirical information.

Since really we know only the values y and W (and their ratio  $\eta$ ) then it is better to re-write Eq. (10) in the form:

$$\sigma T = W + \frac{1-s}{s}y - P_0$$
 where  $s = k(1-r)$ . (12)

If using the relation  $y = \eta W$ , then

$$\sigma T = W(1 - \eta + \frac{\eta}{s}) - P_0 = y(\frac{1}{\eta} + \frac{1}{s} - 1) - P_0.$$
(13)

Let us apply these considerations to the analysis of crop production (maize) in Hungary in 1980s. The necessary data for this system has been taken from Semyonov et al. (1987).

The average yield of maize was 4.9 t/ha (in dry matter) which equals  $0.735 \times 10^{11}$  J/ha. For maize production in Hungary  $\eta = 2.7$  and k = 0.5. The steppe community (Hungarian 'puszta') is a successionally closed ecosystem for a cornfield after cultivation is stopped (grassland of the temperate zone). The gross production of the steppe is equal to  $P_0 = 2800$  kcal/m<sup>2</sup> =  $1.18 \times 10^{11}$  J/ha (Lang, 1990, personal communication). For a maize crop

in the temperate zone  $r \cong 0.4$  (Lang, 1990, personal communication) then s = k(1-r) = 0.3. Substituting these values into Eq. (12) we get  $\sigma T = 0.8 \times 10^{11}$  J/ha. On the other hand, the artificial energy input is equal to  $W = 0.27 \times 10^{11}$  J/ha. Therefore, compensation for environmental degradation requires a 300% increment in energy input with all the additional energy spent only on soil reclamation, pollution control, etc. with no increase in crop production. Note that all the values are calculated per year, i.e. all the values are annual rates of entropy production, of energy production (power), etc.

Let us keep in mind the dynamic equilibrium condition for open systems: the change of its total entropy in the course of characteristic time of the system must be equal to zero. A system, which accumulates entropy, cannot exist for a long time, and it will inevitably be self-destroyed. (Not for nothing the Second Law is the scientific basis of any 'scientific' eschatological concept.) Certainly, we implicitly assume that the considered agroecosystem would be a long living system.

Let us assume that the characteristic time for agriculture is equal to 1 year. (Note that if an agro-ecosystem with crop rotation is considered that the characteristic will be equal to a rotation period, and the entropy balance must be calculated for total rotation.)

The system will be in a dynamic equilibrium and exist an infinitely long time (an entropy does not grow) if  $\sigma = 0$ . Using the part of Eq. (13) containing only W, we get under condition  $\sigma = 0$ :

$$W_{\rm cr} = \frac{P_0}{1 - \eta + \frac{\eta}{s}} = 16 \text{ GJ/ha.}$$
 (14)

Let us compare this value with the values of 'the limit energy load' which have been obtained by Bulatkin (1982) and Novikov (1984) and by Simmons (Zhuchenko, 1988, personal communication). The first two have estimated the 'load' as 14 GJ/ha, while the last has the value 15 GJ/ha. In spite of these estimations having been done from different concepts and considerations, we see that they are very close. Is this not a very curious coincidence? Note that the 'limit energy load' concept is a typically empirical one and it means the maximal value of the total anthropogenic impact (including tillage, fertilisation, irrigation, pest control, harvesting, grain transportation and drying, etc.) on 1 ha of agricultural land. All these values are evaluated in energy units (in accordance with Pimentel's method). It is assumed that when the anthropogenic impact exceeds this limit then the agro-ecosystem begins to be destroyed (soil acidification and erosion, chemical contamination, etc.).

Using the part of Eq. (13) containing only y under the same condition we can calculate (under condition  $\sigma = 0$ ):

$$y_{\rm cr} = \frac{P_0}{\frac{1}{s} + \frac{1}{\eta} - 1} = 2.9$$
 t/ha. (15)

This is an evaluation of the 'sustainable' crop, i.e. the maximal crop production (in dry matter) for 'sustainable' or 'ecological' agriculture.

Let us suppose that the leading, main degradation process, which includes all the degradation processes, is soil erosion. If we have the thermodynamic model of soil erosion, we can estimate the annual erosion losses resulting from intensive agriculture. How to estimate the annual entropy production corresponding to erosive loss of 1 ton of soil? Let us consider soil erosion as a combination of two processes. The first is the burning of organic matter contained in the soil (  $\sim 4\%$  of carbon in mass units), which results in destruction of the chemical structure. The second is a mechanical destruction of soil particles from  $10^{-1}$  to  $10^{-4}$  cm in size. The last is the size of dust particles, which can be weathered by wind and be washed out by water. Then

$$\sigma_{\rm s} T = (0.17 \times 10^{10}) + (0.14 \times 10^{10})$$
$$= 0.31 \times 10^{10} \text{ J/tons.ha.year}$$

where the first item corresponds to chemical destruction and the second to mechanical destruction (Svirezhev, 1990). The annual total erosion loss of soil from 1 ha is equal to  $\sigma /\sigma S = 26$ tons/ha per year. Thus, high crop production will cost us 26 tons of soil loss annually. According to US standards (Odum, 1971), no more than 10 tons of soil may be lost from 1 ha. Obviously, 26 tons per hectare is an extreme value: the actual losses are less, since there are other degradation processes, such as environmental pollution, soil acidification (this factor is very important for Hungary), etc.

There is increasing talk about how chemical 'no-till' agriculture actually allows topsoil to accrete. It is being touted as a 'sustainable' agriculture. Let us consider this concept from the thermodynamic point of view. If you look at the formula for  $\sigma_s T$  you see that the second addendum corresponds to mechanical destruction. The main reason of such destruction is tilling. 'No-till' agriculture means that the value  $\sigma_s T$  is reduced by approximately twice. The first impression is that we achieve our goal and reduce soil erosion. However, it is impossible to get something free of charge, and if we want to have the same crop production we must increase energy input, W, up to the former value replacing the mechanical component by some chemical one. As a result we get approximately the same value of the entropy overproduction,  $\sigma$ , but the result of compensation would be different. For instance, instead of soil erosion we would get an increase of chemical contamination.

Within the framework of the thermodynamic approach we can calculate the entropy of these processes as well. For example, the entropy contribution to the acidification of soil can be calculated in terms of appropriate chemical potentials. However, and this is the principal constraint of thermodynamic approach, we cannot predict the way in which the degradation of the environment will be realised. It may be either mechanical degradation of soil, or chemical pollution, or high acidification of soil, or chemical contamination by pesticides and fertilisers, or others intermediate variants. All ways and all combinations are possible. For the solution of this problem some additional information is needed.

On the other hand, this approach makes it possible to estimate the 'entropy fee', which mankind pays for high crop yield, for the intensification of agriculture. The overproduction of entropy can be compensated by processes of environmental degradation, in particularly, by soil degradation. It is known that the loss of  $\sim 40\%$  of soil results in a rapid, five- to sevenfold decline

in crop yield (Dobrovolsky, 1974). This is a typical agricultural disaster. But it is also a disaster from an anthropocentric point of view, from the point of view of physics, a fall in crop yield through soil degradation is a natural reaction of a physical system, tending to decrease internal production of entropy and to minimise its overproduction. It is the consequence of Prigogine's theorem.

We suspect that there are very serious objections to this statement, especially among biologists, as follows. Certainly, Prigogine's theorem applies to the physical world. The same theorem does not, however, apply to the biological realm, and it is the juxtaposition of the countervailing tendencies of the physical and biological realms that lends tragic overtones to the overwhelming of the biological trend by the physical. In general we agree with this statement but in self-justification we say that we speak as strong followers of reductionism. We understand that this point of view is a biological heresy but we consider an agriculture system only as a physical one. In the framework of our approach we reduce the variety of all the processes inside an agro-ecosystem to the one process of heat production and dissipation. In other words, we measure the entropy production by the total thermal effect of different physical and chemical processes taking place in the system. We understand that it is a very serious simplification of the biological realm but... (how it seems to us) this approach gives some practical results. And it is in this light that we comment on applicability of Prigogine's theorem. The corresponding estimations for Hungary show that if intensive production of maize is continued, agricultural disaster will result in 30-40 years.

#### 4. Systems far from thermodynamic equilibrium

Before introducing some special concepts such as exergy, etc., we must remember that all these concepts consider the ecosystem as a system far from thermodynamic equilibrium. The 'basic' variable for this theory is the rate of entropy production, or the rate of energy dissipation, the so-called the dissipative function ( $\beta$ ). Immediately a series of questions arises, dealing with the behaviour of the dissipative function  $\beta$ .

- 1. How can we calculate the dissipative function  $\beta$  for the system far from thermodynamic equilibrium, if we do not know the appropriate kinetic equations?
- 2. What can we calculate in this case?
- 3. What kinds of 'thermodynamic' statements can be formulated in this case?

We attempt to answer these questions.

Let the dynamics (kinetics) of some biological system be described by the following system of ordinary differential equations:

$$\frac{\mathrm{d}C_i}{\mathrm{d}t} = f_i(C_1, ..., C_n), \quad i = 1, ..., n; \quad C_i \in \mathrm{P}^n, \qquad (16)$$

where  $P^n$  is a positive orthant and  $C = \{C_i\}$  is a vector of state variables.

Let the system in Eq. (16) have a single stable equilibrium point  $\mathbf{C}^* = \{C_i^*\} \in \mathbf{P}^n$ , so that  $\mathbf{C} \to \mathbf{C}^*$  when  $t \to \infty$  for any  $\mathbf{C} \in \mathbf{P}^n$ .

Really, the exact form of equations in Eq. (16) is often not known. In the best case we have a time-series of observations recorded in the course of transition from the initial state  $\mathbf{C}^{\circ} = \{C_i^{\circ}\}$  towards the stable equilibrium  $\mathbf{C}^* = \{C_i^{*}\}$ . It corresponds to the solution  $\mathbf{C} = \mathbf{C}(\mathbf{C}^{\circ}, \mathbf{t})$  of the unknown (to us) basic system of differential equations Eq. (16). Nevertheless, we can calculate the total amount of dissipated energy, L:

$$L = \int_{t_0}^{\infty} \beta(t) \mathrm{d}t$$

for the transition  $\mathbf{C}(t_0) = \mathbf{C}^{\mathbf{o}} \rightarrow \mathbf{C}^*(\infty)$  in one special case.

Let the system dynamics be a movement in a potential field with the chemical potentials  $\mu_i = \mu_{io} + RT \ln C_i$ , i = 1,..., n, where  $C_i$  are molar concentrations of corresponding components and R is the gas constant. Let  $\mu_{10} = \mu_{20} = ... = \mu_{n0}$ , i.e. all the components are substances of identical (or similar) origin. The initial values are arbitrary so that we can consider any point C(t) (except C\*) as an initial point. Since the affinity for reaction

(transition)  $C_i \rightarrow C_i^*$  is equal to  $A_{i,i^*} = RT \ln (C_i / C_i^*)$  then

$$L = \int_{t_0}^{\infty} \beta(t) dt = \int_{t_0}^{\infty} \sum_{i=1}^{n} \beta_i(t) dt$$
  
=  $RT \sum_{i=1}^{n} \int_{t_0}^{\infty} \ln \frac{C_i(t)}{C_i^*} \frac{dC_i}{dt} dt$   
=  $RT \sum_{i=1}^{n} \int_{C_i(t)}^{C_i(\infty)} (\ln C_i - \ln C_i^*) dC_i$   
=  $RT \sum_{i=1}^{n} \{ -C_i \ln \frac{C_i}{C_i^*} + (C_i - C_i^*) \}.$ 

And finally

$$L = \sum_{i=1}^{n} L_{i} = -RT \sum_{i=1}^{n} \left[ C_{i} \ln \frac{C_{i}}{C_{i}^{*}} - (C_{i} - C_{i}^{*}) \right].$$
(17)

You can see that L < 0 for any  $C_i > 0$  (except  $C_i = C_i^*$  when L = 0). It means that for any open system far from thermodynamic equilibrium (when the system moves from a non-stationary state to a stable dynamic equilibrium), the total change of entropy is a negative value. Also, this value does not depend on characteristics of this transition.

On the contrary, spontaneous processes (when the closed system removes to a stable dynamic equilibrium after small internal fluctuations) are accompanied by the increase of entropy. In our case, the transition  $\mathbf{C} \rightarrow \mathbf{C}^*$  is not spontaneous but forced, it depends on the interaction between the system and its environment.

It is obvious that the decrease of entropy (in similar transition processes) is a result of free energy consumption (by the system) from the environment. It is, in turn, a result of exchange processes, which give a negative contribution into the entropy production.

'Revenons à nos moutons', and let us remember formula Eq. (1), which can be re-written in the form

$$\beta = \frac{\mathrm{d}S}{\mathrm{d}t} = \frac{\mathrm{d}_{\mathrm{e}}S}{\mathrm{d}t} + \frac{\mathrm{d}_{\mathrm{i}}S}{\mathrm{d}t}$$

where

$$\beta_{\rm e} = \frac{{\rm d}_{\rm e}S}{{\rm d}t}$$

is a result of exchange between the system and its environment and

$$\beta_{\rm i} = \frac{{\rm d}_{\rm i}S}{{\rm d}t}$$

is a result of internal spontaneous irreversible processes within the system. For 'quasi-equilibrium' systems (the domain of linear thermodynamics, the 'Prigogine World'), $\beta^*$  (and  $|\beta_e^*|$ ) is minimal. Therefore, in similar open systems, when all the transition processes have been finished and one quasi-stationary, 'quasi-equilibrium' state has been established, the 'total energy store' must be minimal.

In our case, for open systems far from thermodynamic equilibrium, the 'total energy store' increases at the expense of exchange between the system and its environment in the course of forced transition to a stable dynamic equilibrium, so that L < 0.

# 5. Exergy and entropy: exergy maximum principle

Let us suppose that the right-hand sides of equations in Eq. (16) depend on some parameters  $\alpha_1, ..., \alpha_m$ , so that

$$\frac{\mathrm{d}C_i}{\mathrm{d}t} = f_i(C_1, ..., C_n; \alpha_1, ..., \alpha_m), \quad i = 1, ..., n.$$
(18)

The vector of parameters  $\alpha$  describes a state of the environment. It is obvious that the equilibrium C<sup>\*</sup> depends on  $\alpha$ . Let us consider the following 'Gedankenexperiment':

- 1. Let the current state of environment be described by the vector  $\alpha^1$ , then  $\mathbf{C}^* = \mathbf{C}^*(\alpha_1)$ .
- 2. We change the environment from the state  $\alpha^1$  to the state  $\alpha^2$  very quickly in comparison with the own time of the system.
- 3. We spend the energy (work)  $E^{12}$  to realise this change.
- 4. After this change the state  $C^*(\alpha_1)$  ceases to be a stationary one, and the system starts to evolve towards a new stationary state  $C^*(\alpha_2)$ .

If calculating the 'dissipative' energy of the transition, we get

$$L^{12} = -RT \sum_{i=1}^{n} \left\{ C_{i}^{*}(\alpha^{1}) \ln \frac{C_{i}^{*}(\alpha^{1})}{C_{i}^{*}(\alpha^{2})} - [C_{i}^{*}(\alpha^{1}) - C_{i}^{*}(\alpha^{2})] \right\}.$$
(19)

Since we cannot cancel the action of the Second Law then  $E^{12} \ge -L^{12}$ ; and min  $E^{12} = -L^{12}$ . We shall consider the extreme case and assume that  $E^{12} = -L^{12}$ .

Let the vector  $\alpha_1$  correspond to the current state of the environment (generally, the biosphere), the vector  $\alpha_2$  correspond to some pre-biological environment and  $\mathbf{C}^*(\alpha_2) = \mathbf{C}^0$  be equal to the concentrations of biogenic elements in some pre-biological structures. Then immediately we get that  $E^{12}$  is nothing more nor less than S.-E. Jørgensen's exergy (Jørgensen, 1992). Therefore

Exergy 
$$(Ex) = RT \sum_{i=1}^{n} \left\{ C_i \ln \frac{C_i}{C_i^s} - (C_i - C_i^0) \right\}.$$
 (20)

Let us remember that the exergy is equal to the work, which is necessary for such a transformation of the system environment, so that in this new environment the system evolves to a pre-biological state. The latter can be considered as a thermodynamic equilibrium, i.e. it corresponds to the death of the system. In other words, the exergy is a necessary energy in order to kill the system, to destroy it.

Note (it is very important) that the work cannot be done on the system directly, it must be done on its environment, i.e. we cannot kill the system directly. In order to do this, we must change the environment in a hostile way (for the system). Therefore, Jørgensen's 'exergy maximum principle' postulates that this work must be maximal.

And finally I would like to call your attention to the following. There is a principal difference between the types of 'Gedankenexperiment' in classic thermodynamics and here. If in classic thermodynamics in order to change the state of the system we perform the work on the system, then in non-equilibrium thermodynamics in order to obtain the same result we must perform the work on the system environment.

### 6. Exergy and information

Introducing the new variables

$$p_i = C_i / \sum_{i=1}^n C_i, \qquad \sum_{i=1}^n C_i = A,$$

where A is the total amount of matter in the system, we can rewrite formula Eq. (20) in the form

$$Ex/RT = A \sum_{i=1}^{n} p_i \ln \frac{p_i}{p_i^0} + \left\{ A \ln \frac{A}{A_0} - (A - A_0) \right\}.$$
(21)

The vector  $p = \{p_1, ..., p_n\}$  describes the structure of the system, i.e.  $p_i$  are intensive variables. The value A is an extensive variable. The expression

$$K = \sum_{i=1}^{n} p_i \ln(p_i/p_i^0) \ge 0$$

is so-called Kullback's measure, which is very popular regarding information measure. Let us consider what the exact meaning of the Kullback measure is (Kullback, 1959) Suppose that the initial distribution  $p^0$  is known. Then we have got some additional information, and, in consequence, the distribution is changed from  $p^0$  to p. So,  $K(\mathbf{p},\mathbf{p}^0)$  is the measure of this additional information. Note that K is a specific measure (per unit of matter). Then the product AK can be considered as a measure of the total amount of information for the whole system, which has been accumulated in the process of transition from some reference state corresponding to a thermodynamic equilibrium, i.e. some 'pre-vital' state, to the current state of living matter.

We can present the expression for the exergy in the form:

$$Ex = Ex_{inf} + Ex_{mat}, \text{ where}$$

$$Ex_{inf} = RTAK(\mathbf{p}, \mathbf{p}^0) \ge 0,$$

$$Ex_{mat} = RT \left[ A \ln \frac{A}{A_0} - (A - A_0) \right] \ge 0,$$
(22)

i.e. as the sum of two terms: the first is a result of structural changes inside the system, and the second is caused by a change of total mass of the system. If we accept Jørgensen's 'exergy maximum principle' then we must postulate that the exergy must increase during the system evolution, i.e.  $dEx/dt \ge 0$  along the system trajectory. Differentiating Eq. (22) in respect to time we have

$$\frac{dEx}{dt} = \frac{dEx_{inf}}{dt} + \frac{dEx_{mat}}{dt}$$
$$= RT \left[ A \frac{dK}{dt} + K \frac{dA}{dt} + \ln \frac{A}{A_0} \frac{dA}{dt} \right]$$
$$= RTA \left[ \frac{dK}{dt} + (K + \ln \frac{A}{A_0}) \frac{1}{A} \frac{dA}{dt} \right].$$

Denoting  $\ln(A/A_0) = \xi$  and taking into account that A > 0 we get the evolutionary criterion in the form

$$\frac{\mathrm{d}K}{\mathrm{d}t} + (K + \xi)\frac{\mathrm{d}\xi}{\mathrm{d}t} \ge 0.$$
(23)

If the positiveness of  $d\xi/dt$  means an increase of the total biomass in the course of evolution then the positiveness of dK/dt can be interpreted as an increase of the information contained in a biomass unit. This, in turn, can be interpreted as a complication of the system structure. If both the complication and the volume (mass) increases then the exergy also increases. If the total biomass is not changed  $(d\xi/dt = 0)$  then the system can evolve only if the complexity of the system structure increases. On the other hand, the structure can be simplified (dK/dt < 0) but if the total biomass grows sufficiently fast  $(d\xi/dt > > 1)$ then the exergy is growing, and the system is evolving. Evolution occurs if the biomass decreases but the structure is becomes complicated (sufficiently fast). At last, there is one paradoxical situation when the exergy is increasing while the total biomass is decreased and the structure is simplified. If  $A < A_0$  then  $\xi < 0$  and  $\xi(d\xi/dt) > 0$ . From Eq. (23) we have

$$\xi \frac{\mathrm{d}\xi}{\mathrm{d}t} \ge \left| \frac{\mathrm{d}K}{\mathrm{d}t} \right| + K \left| \frac{\mathrm{d}\xi}{\mathrm{d}t} \right|. \tag{24}$$

It is obvious that this inequality can be realised if  $|\xi| \gg K$  and  $|dK/dt| \ll 1$ , i.e. the system is sufficiently simple ( $K \ll 1$ ), and the process of further simplification is very slow. Since the condition  $A \ll A_0$  must be fulfilled in order for  $|\xi| \gg 1$  then we can say that the system 'paid' for its own evolution by its own biomass. In the vicinity of thermodynamic equilibrium, at the initial stage of evolution K,  $\xi \sim 0$ . Then from Eq. (23) we get dK/dt > 0, i.e. at the initial stage of evolution the system must complicate its own structure in order to evolve.

### 7. Conclusion

In my presentation I tried to demonstrate how to apply the concepts and methods of classical (and non-classical) thermodynamics to ecological problems. Ecosystems are systems far from the thermodynamic equilibrium and when we try to calculate the entropy by a direct way we immediately get into such difficulties that the solution of the problem becomes very 'problematic'. However, by using the 'entropy pump' hypothesis we can calculate the entropy production for ecosystems under anthropogenic stress by a circuitous way. The entropy can be used as a measure of environmental degradation under anthropogenic impact (for instance, intensive agriculture).

Recently, S.-E. Jørgensen suggested the exergy concept. It is interesting that from the non-equilibrium thermodynamics point of view his concept is one of the possible corollaries of thermodynamic extreme principles. There is a very deep analogy between Jørgensen's exergy and Prigogine's dissipative function.

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