

THERMODYNAMIC MODELING OF BIO-SPECIES ACCOMMODATION

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ABSTRACT

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An ecological model has been constructed. A chemical analogy to the biological system has been developed, and the system's driving forces have been identified.

INTRODUCTION

Theoretical biologists have often indicated the need to identify biological affinities and potentials (Boling, 1973; Ulanowicz, 1972). Biological fluxes are apparent; it is the driving force that has so far seemed elusive. The essence of this research is to develop a chemical analogy to the biological system. The driving forces of the resulting pseudo-chemical system can then be identified. Further, the chemical analog provides a tool with which the effects of disturbances in ecosystems can be easily studied.

BIOLOGICAL MODELING

Fig. 1 illustrates the biological open system, or control volume. The various components are:

- P: primary producer,
- H: herbivore,
- C: carnivore,
- E_h : excretion from herbivore,
- E_c : excretion from carnivore,
- D_h : herbivore dead matter,
- D_c : carnivore dead matter,
- ψ : low entropy external matter,
- W_h : waste matter from D_h reacting with ψ ,
- W_c : waste matter from D_c reacting with ψ .

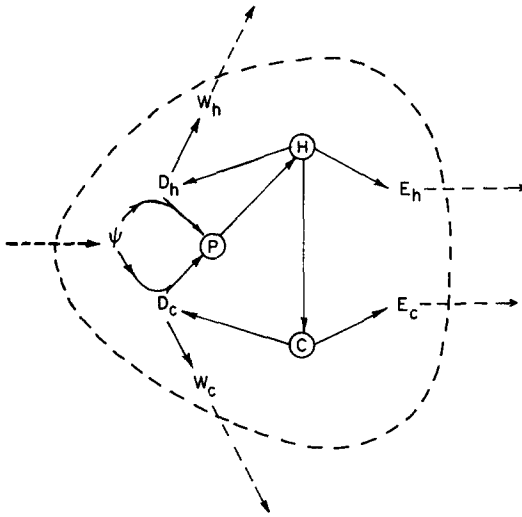


Fig. 1. The control volume.

We have constructed an open ecological system comprised of several species. Our aim has been to include every essential aspect for a physically meaningful ecosystem, and yet keep the complexity to a minimum. This technique can, with no additional conceptual difficulty, be applied to a network having a greater number of species.

P is a primary producer. H is a herbivore which eats P. C is a carnivore which eats H. The dead matter includes parts (cells) of organisms that are replaced in the course of the organisms' maintenance, as well as complete organisms when they die. Excretion is made up of the un-utilized matter from the food intake. The dead matter reacts with the incoming low entropy matter to form primary producer and waste matter. The physical interpretation of such a reaction would be that of a plant growing by taking in carbon dioxide, water vapor, sunlight and fertilizer. The nutrients (fertilizer) would come from the dead matter; ψ would represent carbon dioxide, water vapor and sunlight.

The ecosystem is a control volume containing components which we are interested in studying. As shown in Fig. 2, the control volume is within a system which receives ordered energy (sunlight) and gives off disordered energy (heat). Carbon dioxide and water vapor enter the control volume at a certain state, along with ordered energy (in the form of work which overcomes the concentration gradient, and so forces the carbon dioxide and water vapor into the control volume).

For convenience, the dead matter is assumed to be composed of nutrients; and the excretion and waste matters are assumed to consist of carbon dioxide and water vapor. Thus the nutrients are recycled in the control volume, whereas the carbon dioxide and water vapor flow through the control volume.

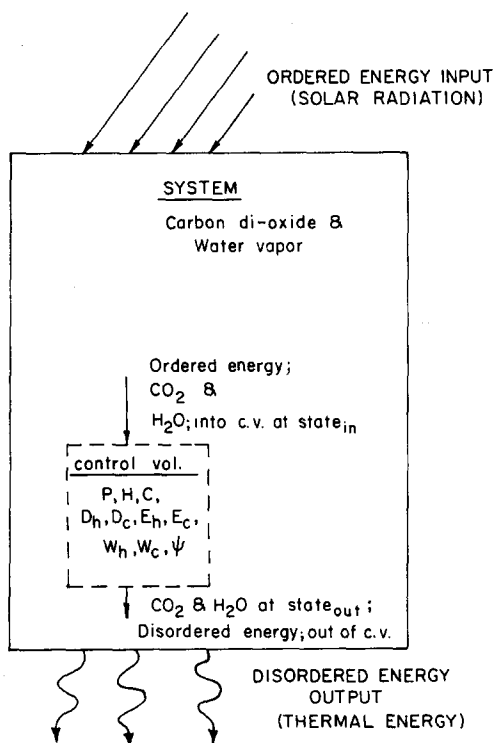
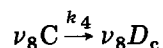
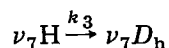
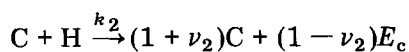
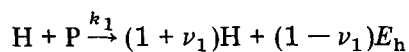


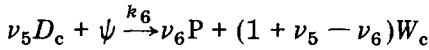
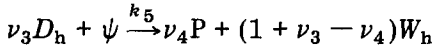
Fig. 2. The control volume within the system.

If the system is large with respect to the control volume, we need not be concerned about the difference in thermodynamic states between the incoming and outgoing flows. The control volume is capable of maintaining its non-equilibrium state because of its being open to these flows; the entropy of the excretion and waste matter flows being much higher than that of the incoming flow of ψ .

THE CHEMICAL ANALOG

The biological system is expressed in the form of the following analogous chemical reactions:





Mass units are used to represent the species in these reactions. In conventional chemistry, moles are used as reaction units. However, the assumption that biological species have approximately equivalent specific volumes is not too bad.

In the case of chemical reactions, the driving force of a reaction j is proportional to the chemical affinity A_j , which is defined in terms of the various stoichiometric coefficients ν_{ji} and the chemical potentials μ_i of the components i in the reaction j :

$$A_j = - \sum_i \nu_{ji} \mu_i \quad (1)$$

$$\mu_i = \mu_i^0 + RT \ln a_i$$

where μ_i^0 is the standard state value of μ_i

$$a_i = \{C_i\} \Gamma_i$$

$\{C_i\}$ is the concentration of i

Γ_i is the activity coefficient (unity for ideal solutions).

Assuming ideal solution,

$$A_j = -(\Delta G^0)_j + RT \ln \prod_i \{C_i\}^{-\nu_{ji}} \quad (2)$$

where

$$(\Delta G^0)_j = \sum_i \nu_{ji} \mu_i^0$$

$$\mu_i^0 = h_i^0 - T s_i^0$$

h_i^0 is the enthalpy of formation of i

s_i^0 is the entropy of formation of i , which can be expressed in terms of the degree of complexity of i thus:

$$s_i^0 = -RT \ln x_i; \text{ where } x_i \text{ is the degree of complexity of } i (0 < x_i < 1).$$

In the following equations the symbols for the components represent the mass concentrations of those components except when used as subscripts. The affinities of the reactions can be expressed in the following manner:

$$A_1 = h_P^0 - \nu_1 h_H^0 - (1 - \nu_1) h_{E_h}^0 + RT \ln \frac{x_P}{x_H^{\nu_1} x_{E_h}^{(1-\nu_1)}} + RT \ln \frac{P}{H^{\nu_1} E_h^{(1-\nu_1)}} \quad (3)$$

$$A_2 = h_H^0 - \nu_2 h_C^0 - (1 - \nu_2) h_{E_c}^0 + RT \ln \frac{x_H}{x_C^{\nu_2} x_{E_c}^{(1-\nu_2)}} + RT \ln \frac{H}{C^{\nu_2} E_c^{(1-\nu_2)}} \quad (4)$$

$$A_3 = \left(h_{\text{H}}^0 - h_{\text{D}_\text{h}}^0 + RT \ln \frac{x_{\text{H}}}{x_{\text{D}_\text{h}}} + RT \ln \frac{\text{H}}{D_\text{h}} \right) \nu_7 \quad (5)$$

$$A_4 = \left(h_{\text{C}}^0 - h_{\text{D}_\text{c}}^0 + RT \ln \frac{x_{\text{C}}}{x_{\text{D}_\text{c}}} + RT \ln \frac{\text{C}}{D_\text{c}} \right) \nu_8 \quad (6)$$

$$A_5 = \nu_3 h_{\text{D}_\text{h}}^0 + h_{\psi}^0 - \nu_4 h_{\text{P}}^0 - (1 + \nu_3 - \nu_4) h_{\text{W}_\text{h}}^0 + RT \ln \frac{x_{\text{D}_\text{h}}^{\nu_3} x_{\psi}}{x_{\text{P}}^{\nu_4} x_{\text{W}_\text{h}}^{(1+\nu_3-\nu_4)}} \\ + RT \ln \frac{D_\text{h}^{\nu_3} \psi}{P^{\nu_4} W_\text{h}^{(1+\nu_3-\nu_4)}} \quad (7)$$

$$A_6 = \nu_5 h_{\text{D}_\text{c}}^0 + h_{\psi}^0 - \nu_6 h_{\text{P}}^0 - (1 + \nu_5 - \nu_6) h_{\text{W}_\text{c}}^0 + RT \ln \frac{x_{\text{D}_\text{c}}^{\nu_5} x_{\psi}}{x_{\text{P}}^{\nu_6} x_{\text{W}_\text{c}}^{(1+\nu_5-\nu_6)}} \\ + RT \ln \frac{D_\text{c}^{\nu_5} \psi}{P^{\nu_6} W_\text{c}^{(1+\nu_5-\nu_6)}} \quad (8)$$

DISCUSSION

The biological interpretation of the rate parameters is worth noting. In conventional chemistry the rate parameters are associated with the time required for the reactants to attain some activated state and the time for the activated compounds to form the products. Biologically, k_1 and k_2 are associated with the time required for H and C (respectively) to become hungry (the hungry state being analogous to the activated state) and the time for satisfying hunger (finding food and eating it); k_5 and k_6 represent a combination of the rates of decomposition (of D_h and D_c respectively), and their subsequent rates of utilization to form P. The death rate parameters k_3 and k_4 are analogous to decay rates. They can be linked to the characteristic life-spans of the organisms, or to some characteristic turn-over rates of the organisms' cells.

The identification of the driving forces [eqs (3)–(8)] is of considerable interest. These affinities are expressed in terms of the concentrations of the various bio-species in the system, and the bio-species' properties of formation. The limiting conditions for the reactions to take place ($A_j > 0$) can be expressed by relating the bio-species' concentrations to their properties. The set ($A_j = 0$) represents equilibrium; and the values of the concentrations satisfying ($A_j = 0$) identify the boundaries of the region ($A_j > 0$). Though the actual living system would be found well within these boundaries, the

absolute limit, beyond which "life" is no longer possible, can be identified. Hence, the "limits of life" may be quantitatively determined.

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