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Modeling Dynamics of Biological and Chemical Components of Aquatic Ecosystems

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MODELING DYNAMICS OF BIOLOGICAL AND CHEMICAL COMPONENTS OF AQUATIC ECOSYSTEMS

by

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ABSTRACT

To provide capability to model aquatic ecosystems or their subsystems as needed for particular research goals, a modeling strategy was developed. Submodels of several processes common to aquatic ecosystems were developed or adapted from previously existing ones. Included are submodels for photosynthesis as a function of light and depth, biological growth rates as a function of temperature, dynamic chemical equilibrium, feeding and growth, and various types of losses to biological populations. These submodels may be used as modules in the construction of models of subsystems or ecosystems. A preliminary model for the nitrogen cycle subsystem was developed using the modeling strategy and applicable submodels.

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SECTION I

CONCLUSIONS AND RECOMMENDATIONS

Models describing the dynamics of complex aquatic ecosystems may be efficiently developed using a five-step systematic approach.

1. Define the aquatic ecosystem in terms of the problem to be solved.

2. Construct a diagram of the ecosystem representing the system variables and the relationship between them.

3. Develop mathematical descriptions of individual physical, chemical, and biological processes involved.

4. Assemble the system model using the submodels while observing the principles of conservation of mass and energy.

5. Compare macroscopic properties of the model with observed properties of the real world to check for validity of the representation.

Although the submodels developed in this report are detailed descriptions of individual ecosystem processes, they may be insufficient to represent some specific natural aquatic systems. Thus, to construct a representation of a given system, submodels for those required processes not covered herein will have to be obtained from other sources or through additional developmental research.

The detailed submodel developed herein, describing biological rates as functions of temperature, provides a representation more useful for ecological models than other available submodels. The fidelity of this function is better over a wide range of temperature than other models examined, provided adequate parameter estimates are obtained.

The nitrogen cycle is a mechanistically complex subsystem of aquatic ecosystems. Within the limitations of the simplifying assumptions used and the lack of good estimates for parameters, the behavior of the model for this cycle was considered to be reasonable. An inhibition function proved to be a key element in the functioning of this model. Properly divided into spatially distinct subsystems and used with reasonable parameter estimates, the nitrogen cycle model will provide a representation of the nitrogen cycle that is suitable for simulation of larger

aquatic ecosystems. Further development work should be done on the nitrogen cycle model to allow it to be included in larger ecosystem models to enhance the capability to predict phenomena related to nitrogen compounds in the environment.

SECTION II

INTRODUCTION

Research on ecological systems, e.g., the fate of pollutants in aquatic ecosystems, may be significantly aided by the use of mathematical models. Such models are frequently thought of as large, complex, relatively incomprehensible computer programs. In fact these programs are not models in the sense used here. A model is a mathematical structure used to represent some real-world process. Computers may be used to make the computations and, in fact, have made it possible to utilize large simultaneous equation models. Computer programs of models permit widespread use and testing of model concepts.

No single model can be general enough to be adequate for every research need. Therefore, our goal is to develop a capability for constructing models to fulfill specific needs that arise in research on the fate of pollutants in aquatic ecosystems.

In the course of working to develop this capability, a systematic approach to the construction of models emerged. To allow construction of models for fate of particular pollutants several terms or equations describing various ecosystem processes were developed or modified from others. These terms or equations, called submodels, may be used as modules in constructing equations that describe rates of change at the population or compartment level. A system of equations that describes the appropriate compartments then may be combined to form a model of some subsystem of a total ecosystem.

SECTION III

THE MODELING PROCESS

The process of constructing mathematical models is more difficult for natural systems than for man-made systems. The former requires an understanding of the way in which nature functions and a knowledge of the functioning units, together with the ability to express the interrelation of these functions in mathematical terms. Although with man-made systems the requirements are similar, the system components are known so that functions are usually understood. For natural systems the essential information may not be available. The element of discovery through scientific inquiry therefore accompanies virtually all modeling of natural systems.

Every mathematical model of ecological systems includes hypotheses that are subject to scientific investigation. In fact a model of ecosystem phenomena may be constructed as a complex hypothesis itself, the hypothesis being that the model is an adequate representation of some aspects of the system behavior as required for a stated purpose. If quantitative outputs are required, the model requires parameter estimates for calibration to a specific situation, and these are obtainable only from data. Only after such calibration can testing begin. The model may be tested relative to another model (is it better?) or against some performance criterion (is it adequate?). Models are neither "good" nor "bad" apart from the purpose they are intended to serve, and testing must be done with this in mind.

PROBLEM DEFINITION

A difficult but signally important step in designing and constructing mathematical models is defining the system to be represented. This definition must consist of at least the set of required outputs, a statement of acceptable error of estimate, and a description of the real-world system generating the analogous real-world outputs. For some purposes other items may be needed, such as identification of controllable variables. With this information modeling may proceed into construction stages.

SYSTEM DIAGRAM

To clarify the relationships among system components it is advantageous to construct diagrams of the systems. Simple block and arrow diagrams may be adequate. Forrester diagrams[1] allow more explicit representation of rates and influencing factors. Odum's[2] energy circuit language may

also be useful. Whatever the scheme, graphical representations allow elaboration of the system from the initial definition to include all identifiable factors of potential significance to the problem.

The system processes and components necessary to provide the required outputs must be represented. The number of these model components depends upon the compromise reached between resolution and economy of resources. It is frequently easier to include many possible components and to delete unnecessary ones later than to begin with a minimal set and add as model development proceeds. Several analytical techniques[3] are available for preliminary analysis of the graphs. These techniques may aid in choosing the optimum set of components to represent the system.

At each stage of model development approximations necessarily are made, each implying some assumption about the real world. All differences between the real world and the model are due entirely to the lack of correspondence between the assumptions and the real world. Results from mathematical analyses of the model may therefore be equated with reality subject only to constraints imposed by the assumptions. Recognition and understanding of the assumptions are therefore necessary to evaluate results from a model.

PROCESS MECHANISMS

For mathematical analysis linear model approximations may be convenient, but when both the pathway of materials and the effects of their concentration are of interest, more complex, nonlinear models will frequently be used. Application of such models requires that the modeler know enough about the processes to construct expressions for the model system variables to adequately describe the interactions among the real-world system entities. Such expressions may merely portray observed behavior at some level of resolution or they may imply complex, real-world interactions that are either hypothesized or known.

In ecosystem models the expressions are used to form terms of the equations. Whereas the terms represent interactions, the equations represent real-world components such as populations, aggregations of similar populations, or trophic levels. Especially where the functional groupings represent entities such as populations or groupings of similar populations, the form of the terms is determined by the way the modeler mathematically describes the physiological or kinetic properties of these interacting real-world entities. For any interaction the term must appear in at least two equations, often called donor and

recipient equations (e.g., predator and prey). The term in a particular equation takes an appropriate sign and is modified by coefficients for efficiency of transfer (utilization, etc.) and for stoichiometry. Letting D = donor and R = recipient, assuming a simple rectangular hyperbolic description of growth of R on D, and expressing them in like units, such an interaction can be illustrated as follows:

$$\frac{dD}{dt} = -\frac{\hat{\mu}R}{Y}\left(\frac{D}{K+D}\right) + \cdots$$

$$\frac{dR}{dt} = \hat{\mu}R\left(\frac{D}{K+D}\right) + \cdots$$

where $\hat{\mu}$ = growth rate constant

K = constant for half-maximal growth rate of R on D, and

Y = yield of R per unit of D consumed, $0 < Y \leq 1$.

The term $\hat{\mu}D/(K + D)$ describes a simple "physiology" of R with respect to D. The interaction is described by the couple, i.e., the appearance of the term in both equations.

In summary, modeling ecosystems using a mechanistic approach involves writing equations, each of which consists of terms that appear in one or more equations. The couples (or n-tuples) of terms represent interactions, and they are constructed so as to describe the physiology or kinetics in the detail appropriate to the problem. No matter how complex, all models are approximative. They may therefore be judged only by their value after application to their intended purpose.

PHYSICAL CONSTRAINTS - CONSERVATION OF MASS AND ENERGY

Ecological systems are constrained in nature by the availability of matter and energy. Models of such systems must be constrained by analogous physical principles. Mass and energy budgets must be maintained if models are to be realistic with respect to principles of conservation of mass and energy.

In the preceding example of an interaction, another equation is required for conservation of mass. The loss of donor is proportional to μ/Y, but gain by recipient is proportional to μ alone. Hence an amount proportional to

(1/Y)-1 is unaccounted for. Another equation for a by-product, B, will account for all the mass:

$$\frac{dB}{dt} = \hat{\mu}R\left(\frac{1}{Y} - 1\right)\left(\frac{D}{K+D}\right) + \ldots$$

The equation for the by-product may be ignored when it is of no interest to the model.

The most important benefit of the principle of conservation of mass in modeling is the realistic constraint that it places upon model behavior. In the above example by-product accumulates as donor disappears and as recipient increases. Because total mass remains constant the changes in the three components are correctly phased in time. In general the mass balance constraint ensures correctly phased behavior of model components, an important characteristic of ecosystem models.

USE OF MODELS

Simulation, the calculation of system behavior as a function of time, and mathematical analysis may be used to examine or analyze models for their properties. Models are analyzed for two basic reasons. In their development, analysis is done to compare macroscopic properties of the model to known properties of the real-world system to check for misrepresentation. When the model has been judged to be an accurate representation of the real world for the purposes intended, it is analyzed to seek properties of the real system by observing properties of the model. For a complex nonlinear model mathematical analyses may be difficult or impossible, and therefore examination of simulation results is the more frequently used approach. Simulation is frequently used to obtain responses of the model to specific conditions, i.e., answers to "what if" questions.

The constituent submodels can also be used separately if information about a single subcompartment only is needed, e.g., chemical equilibrium or accumulation of toxic substances in an organism. Such computations may also be done as a preliminary check on parameter values before doing a large simulation.

A model may serve as a complex hypothesis about the real world. It can be used to plan experiments, the goal of which is to provide data to modify the model, if necessary, to better describe the real world.

Models discussed are structured in detail to facilitate research, but future models may be made simpler by using generalizations obtained from research suggested by the detailed models. Simplifying assumptions are frequently made because of insufficient knowledge, but simplifications resulting from research insights can lead to more useful and reliable models.

SECTION IV

PROCESS MODELS

Many different strategies are used to construct ecosystem models. Process modeling is one such strategy. In it, mathematical expressions are constructed to describe mechanistically at some chosen level of resolution the various processes taking place in the real world, e.g., transfer, transformation, birth, and death. These expressions, termed submodels, may then be used as modules in the construction of larger subsystem, ecosystem models.

The processes are described mechanistically, to permit valid predictions beyond the range of the calibration data where mechanisms are understood, and to permit incorporation of testable hypotheses where they are not.

RESPONSE OF BIOLOGICAL RATES TO PHYSICAL FACTORS

The physical factors of light and temperature are important environmental variables in ecosystems. Because the process of photosynthesis is the basic biochemical reaction supporting life it is important to pay particular attention to its description in constructing a mechanistic model for an aquatic ecosystem. Accurate computation of the rate of primary production of organic material, especially for lakes or slowly flowing water bodies, is necessary for accuracy in other computations related to living organisms.

Temperate zone temperatures vary widely through the seasons. Simulations of ecosystems over long time intervals therefore require accurate descriptions of responses of various rates to temperature changes.

Algal Growth as a Function of Light

Light is one of the principle factors affecting plant growth. Because many of the materials frequently dissolved or suspended in aquatic systems absorb or scatter light, light entering at the surface is attenuated as it penetrates the water. Light intensity therefore is a function of depth and of water content. Hence, in modeling the response of an aquatic ecosystem to light, absorption and turbidity must be included. Because plant pigments are sensitized by light of discrete wavelengths, it may be necessary to include expressions for the differential light absorption characteristics of the various materials present.

The influence of light was represented in two ways. The simplest was to use a scaled and truncated sine wave as a

crude means of describing algal growth as it varies with light intensity throughout the daylight cycle[4].

Hutchinson[5] presented a more explicit representation of light penetration using an integrated form of Beer's Law. It includes direct light absorption by water and absorbing materials (color), and attenuation by scattering particulates. Light intensity I at depth z may be expressed as

$$I_z = I_o e^{-(\eta_w+\eta_c+\eta_p)z} \quad (1)$$

where I_o = intensity at the surface,

η_i = extinction rates per unit depth, (products of an extinction coefficient and concentration of the light adsorbing substance, indicated by subscript i:

w = water,

c = color,

P = particulate turbidity.

The extinction rates for color and turbidity vary widely. The rate for particulate turbidity may be written as $\eta_p = hP$ where P is a turbidity measure and h is an extinction coefficient. P may be subdivided into turbidity by non-living and living particles. If the non-living particles can be assumed constant with time for a particular situation and the light-absorbing living particles are all algae, then the equation has only one variable, algal density. Separating the algal density from the density of non-living particles, the expression for the exponential extinction rate, η_T, becomes

$$\eta_T = (\eta_w + \eta_c + h_n P_n + h_e \Sigma_i C_i) \quad (2)$$

where C_i = the concentration of chlorophyll a in the ith group of algae (mg m^{-3}),

$h_n P_n$ = the extinction rate for non-living particle turbidity, and

h_e = the extinction coefficient for chlorophyll a.

A further modification of the equation for I_z incorporating the non-vertical light path results in

$$I_z = I_o e^{-1.19\eta_T z} \quad (3)$$

in which 1.19z is the distance traveled by the average beam of light in reaching depth z. Poole and Atkins[5] found the factor 1.19 to apply throughout the day because of the varying contribution to the total incident light by direct sunlight and by skylight.

To assess the integrated effect of light on the growth of a population of photosynthesizing cells dispersed throughout a water column of the euphotic zone, a function relating growth rate to light intensity is needed. Steele[6] presented such a model for photosynthesis as a function of light intensity as follows:

$$p = ap_m Ie^{1-aI} \quad (4)$$

where a is a scaling constant, and

p_m is maximum photosynthesis rate.

No rationale or development for the model was presented, but the equation fits several sets of photosynthesis-light curves.

The equation can be derived from the following:

1. The rate of change of p with a unit change in I depends both on the value of p and on the deviation of I from the optimum I (I_m);

2. The rate of change of p with a unit change in I is inversely proportional to I, i.e., the photoinhibition effect.

The following equation expresses these assumptions:

$$\frac{dp}{dI} = \frac{kp\ (1-I/I_m)}{I}$$

Integration yields the following:

$$p = p_m (I/I_m)^k e^{k(1-I/I_m)} \quad (5)$$

Steele's[6] equation (4) is obtained by letting $k = 1$ and $1/I_m = a$. Equation (5), because it contains the parameter k, which can be fit to data, provides a better fit than does Steele's equation. However, the form of Steele's equation, because of its tractability, is more useful in developing expressions for the average growth in a water column. When equation (5) was fit by least squares to widely differing data sets, k varied from about 0.87 to about 1.67. For wide variation in light intensities, computations using equation (5) will give better results than will equation (4).

Steele's equation may be integrated over the depth of the euphotic zone (or other chosen depth) in order to obtain the average photosynthesis rate. Substituting equation (3) into equation (4), integrating over the depth, z_e, of the euphotic zone, and averaging, the necessary expression is obtained

$$\bar{p} = \frac{p_m}{1.19\ \eta_T z_e} \int_0^{z_e} \left(e^{1 - I_o/I_m e^{-1.19\eta_T z}}\right)\left(\frac{1.19\eta_T I_o}{I_m}\ e^{-1.19\eta_T z}\right) dz$$

$$\bar{p} = p_m \frac{\left(e^{1 - I_o/I_m e^{-1.19\eta_T z_e}} - e^{1 - I_o/I_m}\right)}{1.19\ \eta_T z_e} \tag{6}$$

Bannister[7] discussed the variable nature of p_m and the relatively constant nature of another parameter ϕ_m, the maximum quantum yield. Using Steele's equation Bannister[7] derived p_m in terms of ϕ_m and C (mg chlorophyll/m³):

$$p_m = 12\ \phi_m\ I_m\ h_c\ C/e$$

where 12 = atomic weight of carbon, and

h_c = the rate of absorption of light by chlorophyll a.

Substituting Bannister's expression into equation (6) gives $\bar{p}$ in terms of I, C, and the parameters η_T, ϕ_m, I_o, and I_m:

$$\bar{p} = \frac{12\ \phi_m I_m h_c C \left[e^{-I_o/I_m e^{-1.19\eta_T z_e}} - e^{-I_o/I_m}\right]}{1.19\ \eta_T z_e} \tag{7}$$

This expression assumes that all algae are alike. The average rate of photosynthesis for the jth algal group is $(\overline{p} \cdot C_j/C)$. Therefore the expression for the rate of photosynthesis by the jth group is

$$\overline{p}_j = \frac{12\ \phi_m I_{mj} h_c C_j \left(e^{-I_o/I_{mj} e^{-1.19\eta_T z_e}} - e^{-I_o/I_{mj}}\right)}{1.19\eta_T z_e} \tag{8}$$

This expression can be used for simulations or other computations utilizing the average photosynthesis rate for a column of euphotic zone water under a meter square of surface. However, an expression for the rate of carbon fixation per unit biomass, π, is usually more convenient for simulation. To obtain an expression for π using equation (8), a relationship between chlorophyll and biomass (B) is needed:

$$C_j = b_j B_j$$

where b_j = chlorophyll per unit biomass of population j.

Substituting for C and dividing by B gives

$$\pi_j = \frac{12\ \phi_m I_{mj} h_c b_j \left(e^{-I_o/I_{mj} e^{-1.19\eta_T z_e}} - e^{-I_o/I_{mj}}\right)}{1.19\eta_T z_e}$$

Finally the specific growth rate subject only to light limitation, $\hat{\mu}'$, must be obtained in terms of π and the stoichiometric coefficient relating total biomass to carbon, n_a:

$$\hat{\mu}' = n_a \pi \tag{9}$$

The relationship of $\hat{\mu}'$ to the specific growth rate, μ, in the context of nutrient and temperature limitations will be discussed separately and a tentative expression for μ will be developed in a following section.

In the above discussion only phytoplankton dispersed uniformly throughout the water column are considered. Other kinds of plants are also important in aquatic ecosystems. In fact, in streams attached algae and rooted macrophytes may account for the entire productive capacity. A development similar to the one above would result in an expression similar to equation (9) for the growth of macrophytes. Whereas uniformly dispersed phytoplankton are easily represented in equations for light extinction, discrete leaves of macrophytes may cause some problems in representation. However, a term for total leaf area could be used as a light extinction variable as described by Bloomfield et al.[8] in a model describing macrophyte growth in an ecological context.

Biological Rate as a Function of Temperature

Temperature is a principle abiotic factor in providing niche requirements for organisms. The existence of upper and lower limits outside which biological processes fail points to the likelihood of a temperature response with a optimum for these processes.

Much of the work with biological rates as functions of temperature makes use of the concept of Q_{10}. Q_{10} is the ratio of rate constants of biological reactions at two temperatures, 10 degrees apart. Assuming that the rate is exponentially related to temperature over the interval of interest, the following expression[9] describes the relationship between rate constants and temperatures:

$$Q_{10} = (k_1/k_2)^{10/(T_1-T_2)}$$

where T_1 and T_2 may differ by any amount.

Given a Q_{10} value and a rate constant (k_1) at some temperature (T_1), one can determine the rate constant, k_2, at some other temperature, T_2.

$$k_2 = k_1 \, Q_{10}^{(T_2-T_1)/10}$$

However, the assumption that the rate increases exponentially with temperature is not valid over a large portion of the range of temperatures that an organism will tolerate. Instead the biological rate increases with increasing temperature to a maximum at an optimum temperature (T_m),

then falls off to zero at some upper limiting temperature (T_L).

Three different sub-models or equations have been developed to describe the dependence of biological rates on temperature, all of which are characterized by a temperature optimum with an associated maximum rate. One was developed for use in ecosystem models for the Eastern Decidious Forest Biome of the International Biological Program (IBP)[8]. Its form is rather complex:

$$k = \left(\frac{T_L - T}{T_L - T_m}\right)^X e^{X[1 - (T_L - T)/(T_L - T_m)]} \tag{10}$$

where $X = \dfrac{W^2[1 + \sqrt{(1 + 40/W)}]^2}{400}$

$W = (\ln Q_{10})(T_L - T)$

and all other symbols are as previously defined.

Since it contains only two parameters and a Q_{10}, this model is not able to represent rates over a wide variety of temperatures. However, it is useful around the optimum temperature.

A second equation was presented by Johnson et al.[10]. Based upon transition state theory, this model assumes that the rate of an enzyme reaction is a function of the activation energy and the equilibrium between the native and denatured forms of the enzyme. It has the form

$$k = \frac{c\,T\,e^{-\Delta H\ddagger/RT}}{1 + e^{\Delta S/R - \Delta H/RT}} \tag{11}$$

where c is a scaling constant,

$\Delta H\ddagger$ is the heat of activation for transition state intermediates,

ΔH is the heat of activation for the reaction for which k is the rate coefficient,

ΔS is the entropy of activation of the same reaction, and

R is the gas law constant.

This model may be fit to biological rates over wide temperature ranges; however, its parameters are thermodynamic quantities, which are difficult to interpret at the ecological level.

Another model, presented by Lassiter and Kearns[4], was developed in response to a need for a simple model, applicable over a wide temperature range. The model takes into consideration the following factors:

- Rate coefficients are always positive, approaching zero asymptotically with respect to values of an external stimulus; thus a change in the rate in response to an external stimulus must be proportional to the magnitude of the rate itself.

- A biological rate constant reaches maximum at an optimum temperature; therefore, the rate of change of the constant is hypothesized to be proportional to the deviation of temperature from optimum.

- The rate, which diminishes when the optimum temperature is exceeded (its rate of change becomes negative), decreases more rapidly as the upper limit is approached. An inverse relationship between the rate of change and deviation from the maximum temperature (T_L) is hypothesized.

The following equation incorporates the above considerations:

$$\frac{dk}{dT} = \frac{a\ k\ (T_m - T)}{(T_L - T)} \tag{12}$$

Integration of equation (12) with $k = k_m$ when $T = T_m$ results in the following expression[4]:

$$k = \begin{cases} k_m \left[e^{a(T-T_m)} \right] \left(\frac{T_L - T}{T_L - T_m} \right)^{a(T_L - T_m)} & , T \leq T_L \\ 0 & , T > T_L \end{cases}$$

Although the equation contains four parameters, it fits only data that conform generally to the assumptions used to derive the equation. The graph of the equation is always skewed to the right (Figure 1), the amount of skew depending upon the difference between T_m and T_L. No other type of data can be represented by the model.

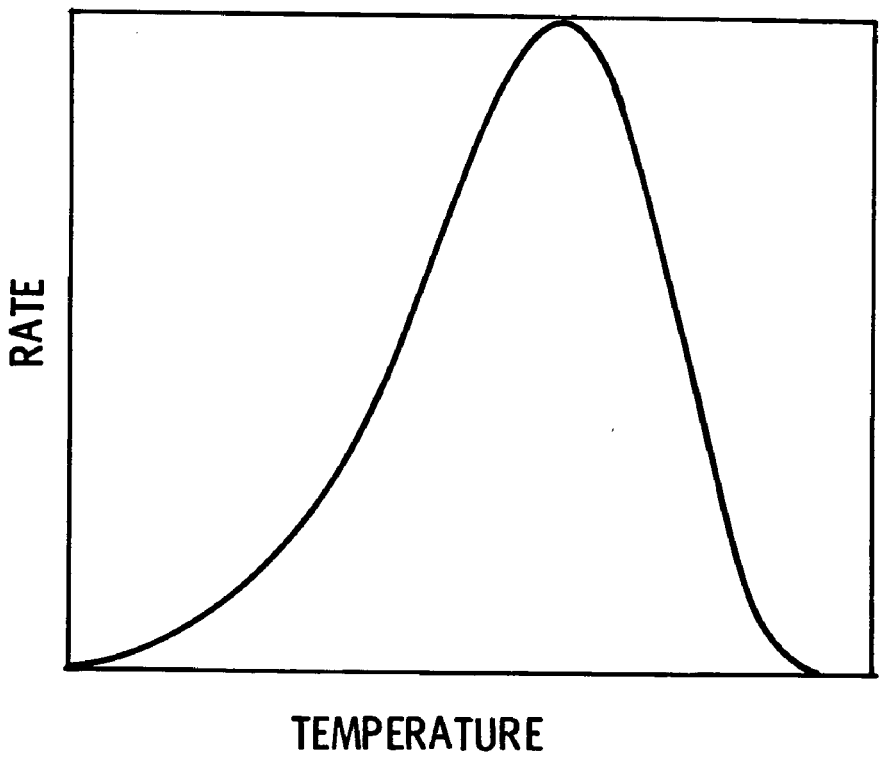

Figure 1. General shape of the graph of biological rate versus temperature as described by equation (13).

The model has been fit to several sets of published data, e.g., growth rates of Chlorella sp.[11], egg production by several species of wood fungi[12], growth of four species of aquatic snails[13], and luminescence from certain luciferin/luciferase reactions[10]. Figures 2 through 4 give examples of fits to published data. The equation is a good representation for all data thus far examined on biological rates versus temperature.

The shape of the graph for the equation is similar to that for equation (11). Figures 5 and 6 show least squares fits of equations (11) and (13) to the same data set (Figure 8.25, Johnson et al.[10]). The fits are not markedly different. Equation (11) may be more meaningful in an analytical sense in that parameters are thermodynamic quantities, which permit biological rates to be compared on fundamental grounds. However, for ecological modeling it may be more meaningful to use the parameters of equation (13) for the function relating growth or other biological rate to temperature.

Because Q_{10} data have been so frequently reported, they represent a source of information that may be used in deriving the parameters for equation (13). For example, given a Q_{10} computed from rates obtained over the temperature range T_1 to T_2 and reasonable estimates for T_m and T_L, values for k_m and a may be computed.

Using the two rates k_1 at T_1 and k_2 at T_2 or any two rates in the range over which Q_{10} is valid, and the estimates of T_m and T_L, the constant, a, may be computed by the following equation:

$$a = \frac{\ln k_1 - \ln k_2}{(T_1-T_2) + (T_L-T_m)\ \{\ln[(T_L-T_1)/(T_L-T_2)]\}} \qquad (14)$$

The optimum rate, k_m, may then be computed by substituting a into equation (13) with $k = k_1$ at T_1 or $k = k_2$ at T_2. Using k_1 and T_1, the following expression may be used to determine k_m:

$$k_m = k_1 e^{-a(T_1-T_m)} [(T_L-T_1)/(T_L-T_m)]^{-a(T_L-T_m)} \qquad (15)$$

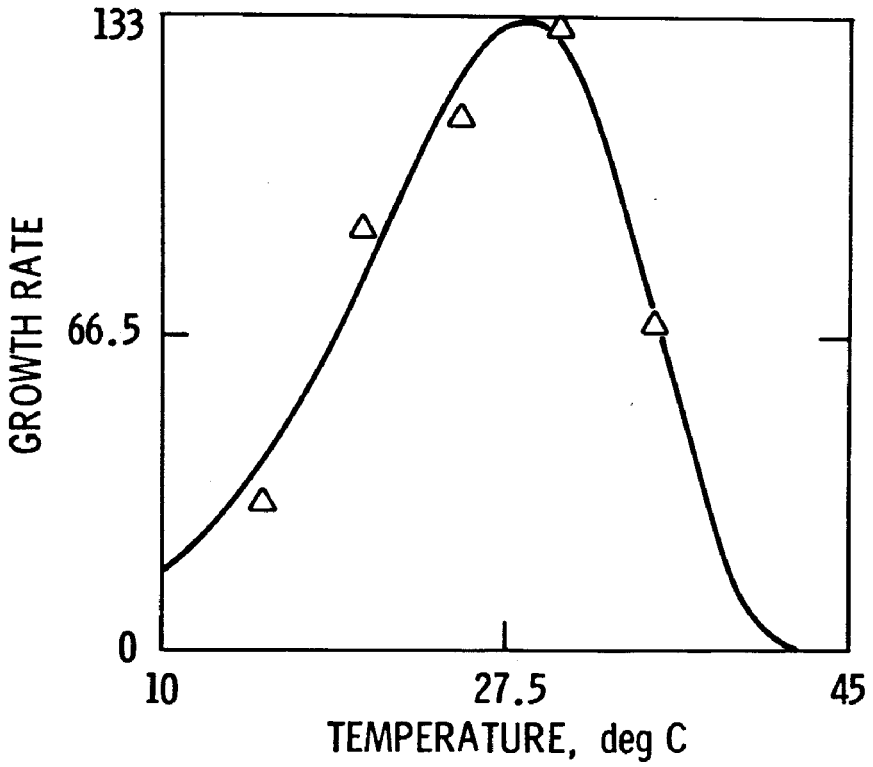

Figure 2. Fit of equation (13) to data for growth rate of the planktonic green alga, Chlorella pyrenoidosa, over a temperature range.

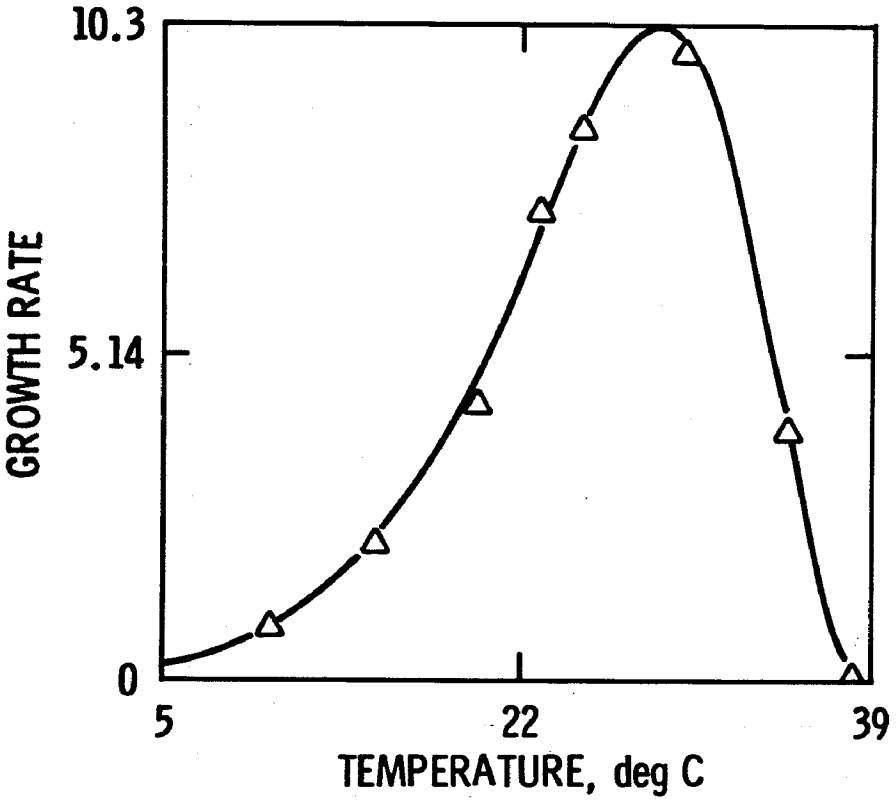

Figure 3. Fit of equation (13) to data for growth rate of the wood destroying fungus, Ganoderma aplanatum, over a temperature range.

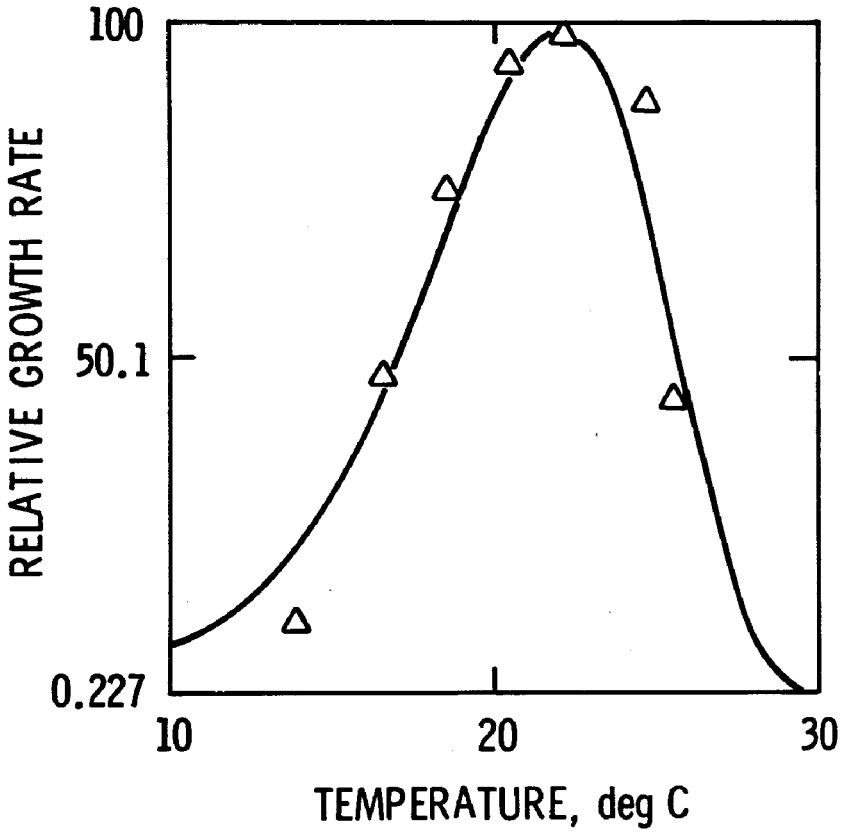

Figure 4. Fit of equation (13) to data for growth rate of the aquatic snail, Lymnaea stagnalis, over a temperature range.

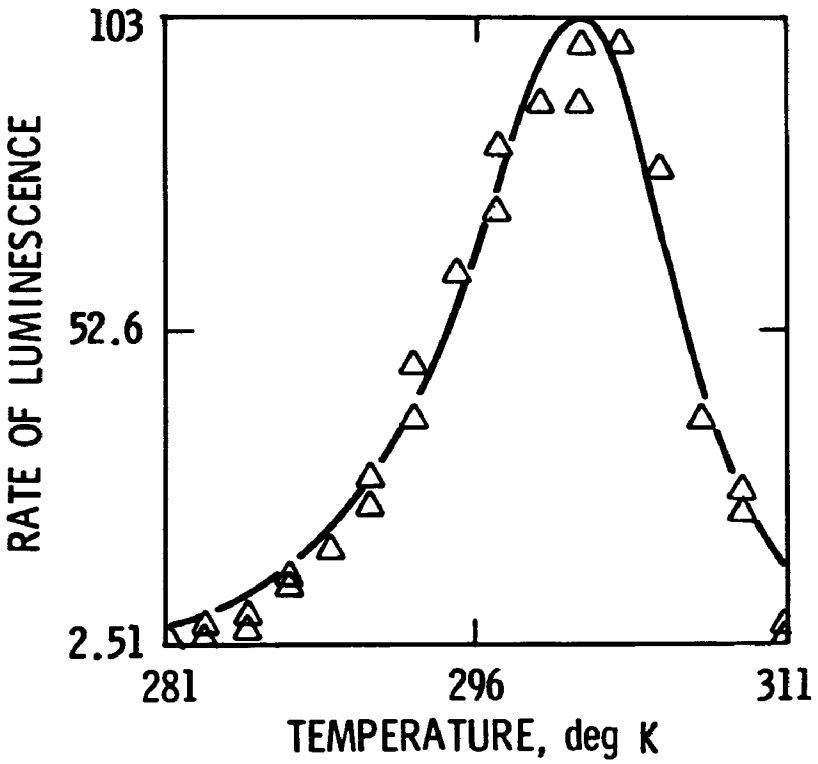

Figure 5. Fit of equation (11) to data of rate of luminescence in the luciferin-luciferase system over a temperature range[10].

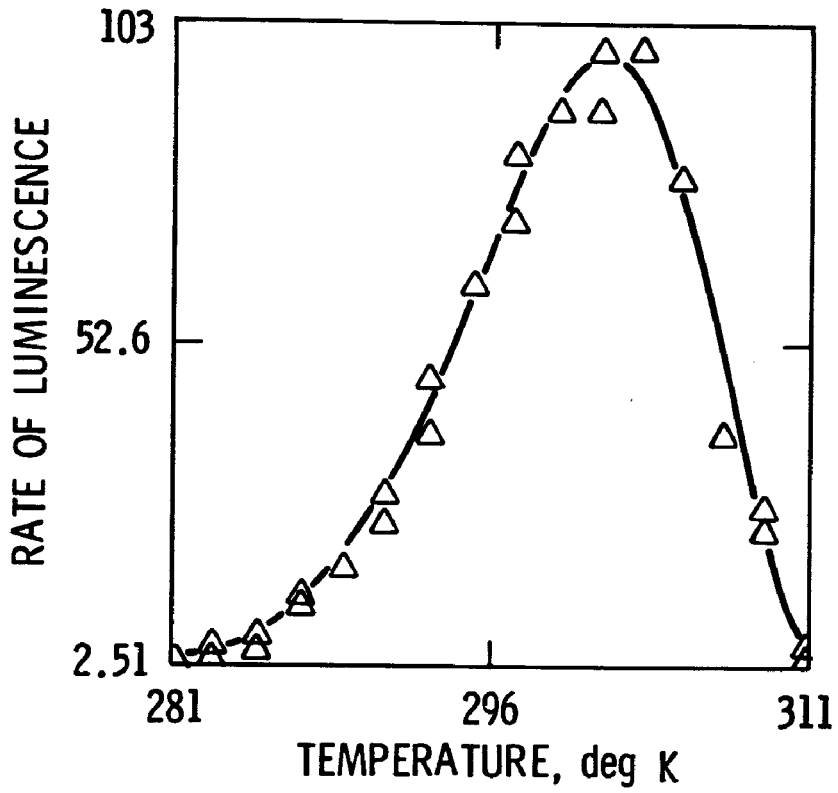

Figure 6. Fit of equation (13) to data of rate of luminescence in the luciferin-luciferase system over a temperature range[10].

To solve equation (13) for all four parameters, rates at four temperatures are needed.

If a larger set of data for rate versus temperature is available, the parameters may be better estimated by least squares. This technique[14] was used to fit the equation to the growth, egg production, and luminescence data cited previously.

For modeling aquatic ecosystem processes, equation (13) is easily used and has been found to describe adequately the response of rate processes to temperature fluctuations.

INTERACTIONS OF ORGANISMS AND THEIR CHEMICAL ENVIRONMENT

The biota are controlled by the availability of chemicals and the chemicals in turn are transformed by the organisms[21]. A description of the ecosystem therefore requires a set of simultaneous differential equations for both biota and chemicals, all highly coupled.

The biota influence their physical environment in simple ways such as reducing light intensity by shading. Biological and chemical processes, however, seem to be linked in much more complex and subtle ways. Many chemical reactions occur so rapidly that they may be considered to be always at equilibrium with respect to the much slower biological processes. Yet these biological processes over a period of time may exert a great influence on the chemical system. The molar ratio (16:1) of nitrogen to phosphorus in the sea is presumably an example of such influence resulting from biological processes operating over geological time[15].

Descriptions of several processes involving interactions between the biota and their chemical environment were included as components for the ecosystem models:

- inorganic chemical equilibrium
- production and decomposition of organic compounds,
- exchange of gaseous materials at the air-water interface, and
- food-web transfers of the aquatic biological community.

Figure 7 shows schematically components and transfers that are important in biogeochemical cycles. Although pollutants are generally thought of in terms of their effects on the environment, a model for the fate of pollutants must in addition consider them as materials subject to transfer and transformation by the above processes.

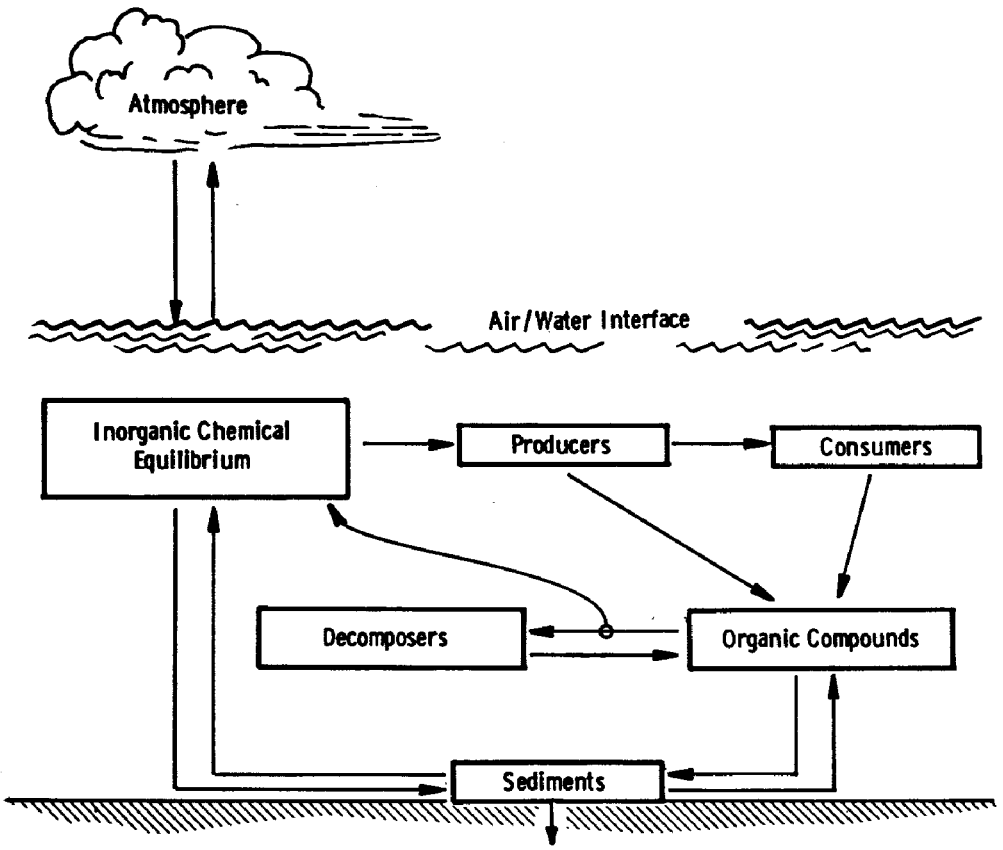

Figure 7. Components and transfers important in biogeochemical cycles.

Dynamic Chemical Equilibrium

The dissolved materials in aquatic systems comprise a complex medium wherein photochemical, biochemical, and other chemical processes occur. It is beyond the scope of most dynamic models to represent this complexity in more than a simple way.

To develop a capability to model chemical equilibria dynamically, a simple representation of the complex real world was chosen that would include materials of rather certain importance to ecosystem processes. Various techniques have been presented for computing concentrations of materials in complex solution equilibria[16,17,18], but for this submodel a simpler computational scheme was needed that would allow the chemical equilibria to be maintained dynamically throughout a simulated time period. The technique chosen was an iterative search for $[H^+]$ that results in achievement of charge balance.

Ionization fractions or distribution coefficients as functions of the equilibrium constants and hydrogen ion concentration were computed for each ligand. For example the carbonate series is characterized by three distribution coefficients, α_0, α_1, and α_2:

$$\alpha_0 = \frac{[H_2CO_3^*]}{C_T} = \left(1 + \frac{K_1}{[H^+]} + \frac{K_1K_2}{[H^+]^2}\right)^{-1} ,$$

$$\alpha_1 = \frac{[HCO_3^-]}{C_T} = \left(\frac{[H^+]}{K_1} + 1 + \frac{[K_2]}{[H^+]}\right)^{-1} ,$$

$$\alpha_2 = \frac{CO_3^=}{C_T} = \left(\frac{[H^+]}{K_1K_2} + \frac{[H^+]}{K_2} + 1\right)^{-1} ,$$

where $C_T = [H_2CO_3^*] + [HCO_3^-] + [CO_3^=]$

$[H_2CO_3^*] = [CO_2] + [H_2CO_3]$.

The α_i are found simply by substituting a value for $[H^+]$.

Given a distribution coefficient, α_i, and the total concentration, C_T, the concentration of any form, C_i, can be computed:

$$C_i = \alpha_i C_T$$

Distribution coefficients are used in this manner to compute the concentrations of all the ligands considered. Concentrations of the free metal ions are computed using concentrations of the ligands and solubility products, subject to the constraint that the total metal present remain constant. If computation indicates precipitation, the solids are assumed to remain in microdispersed form, readily available for solution when conditions permit. The key to all computations is $[H^+]$. $[H^+]$ is varied by the iterative search routine until the objective function, a net charge equation, is found to be arbitrarily close to zero, at which point the computations are complete.

For the chemical equilibrium system to be maintained dynamically, the totals of materials used and regenerated may be changed each computational interval. Differential equations for CO_2, available phosphate, and NH_3 (discussed later) are used to compute these additions and subtractions.

The largest set of metals and ligands utilized included sodium, calcium, magnesium, carbonates, phosphates, sulphates, sulfide, acetate, ammonia, and nitrate. Equilibrium constants were obtained from various sources including Kern[19] and Stumm and Morgan[15].

Aquatic ecosystems were simulated using the model of Lassiter and Kearns[4] with and without chemical equilibrium. The pattern of biomass production, especially for primary producers, was different for the two cases. Without chemical equilibrium only one form of a chemical nutrient could be assumed, and therefore as might be expected, growth of producers and corresponding depletion of the nutrient proceeded faster. When the model included chemical equilibrium, the chemical nutrients were apportioned among several chemical species with a corresponding lowering of the concentration of the available form. As the chemicals were used they were reapportioned by equilibration and therefore made available in a buffered fashion to the organisms.

Variation in pH was induced by the algal growth components in the model similar to the manner in which it occurs in nature. One curve presented[4] showed an abrupt halt in pH fluctuations with the development of phosphorus limitation. Another simulation with higher decomposition rates (higher rate of mineral recycling) also resulted in low phosphorus concentrations terminating a bloom. However, with the higher recycling rates the pH fluctuations did not abruptly cease, but instead decreased rapidly in magnitude. These results are shown in Figure 8.

Both studies illustrate the importance of a dynamically varying chemical equilibrium subsystem as part of models directed toward study of nutrient-algal relationships. The

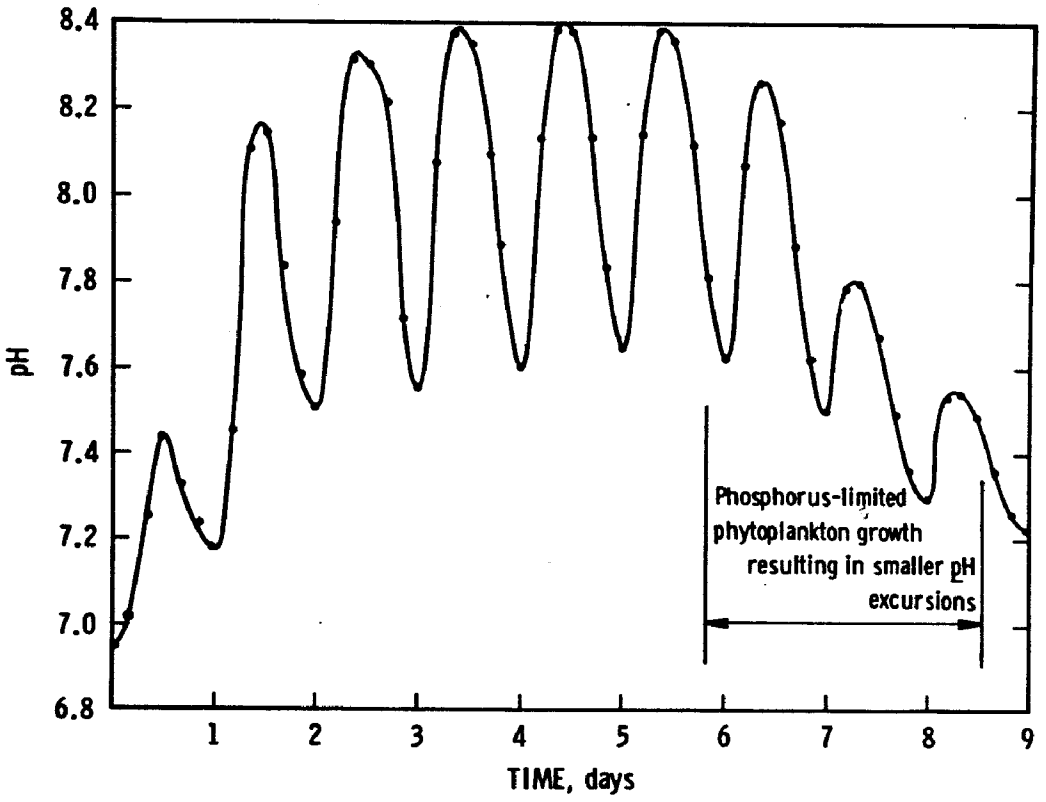

Figure 8. Pattern of pH fluctuations during course of algal bloom and termination of the bloom by phosphorus limitation. Smooth curve was drawn through points (dots) produced by a computer program for a dynamic chemical equilibrium model linked to a differential equation model of phytoplankton dynamics.

fluctuations in pH are as much a part of these relationships as are the fluctuations in either nutrient concentration or algal density, and perhaps carry greater implications for other, less directly related, reactions such as those of specific pollutants.

The chemical equilibrium submodel has two major disadvantages. First, equilibrium constants have not been corrected for temperature. Falls and Varga[20] list some of their equilibrium constants as functions of temperature, and data such as these will be useful. Second, the method is not general enough to allow relative ease of specification of the system. The system described above will probably be abandoned and replaced by a streamlined subset of another model such as that presented by Morel and Morgan[17], which overcomes at least the latter problem. The use of the present system has, however, provided experience with a dynamic equilibrium model, and its use has shown that it is feasible to represent dynamic chemical equilibria concurrently with biological processes in ecosystem models.

Microbial Growth

One important microbial activity in ecosystems is decomposition, the recycling of nutrients from organic back to inorganic forms. A representation of this feature of the ecosystem is necessary in models that are intended to accurately represent the cycling of materials[21]. Decomposition is a function of growth rate, and therefore an expression for microbial growth is needed.

Microbes in general (algae and bacteria for present purposes) require for growth an energy source, inorganic nutrients, and a suitable chemical and physical environment.

For algae, which are autotrophic, the energy source is light, a physical factor (discussed previously). An equation was derived for algal growth as limited by light (energy) alone (equation 9). Bacteria, because they feed on non-living organic material, are considered to be not only heterotrophic, but more specifically, saprophagous[22]. They derive their energy from the transformation and utilization of organic materials. Before an equation can be derived that describes microbial growth in general as a function of inorganic nutrient concentrations, an expression for bacterial growth as limited by energy sources, analogous to equation (9) for algae, must be developed.

One approach to the development of an equation for bacteria is to consider free energy changes in net equations for the transformation of particulate organic matter into bacterial biomass. Assume that the organic material in the system may assume four different forms -- particulate

organic matter (OM_p), dissolved or broken down organic matter (OM_d), oxidized organics (CO_2 and other inorganic ions), and bacterial biomass. The free energy changes associated with the transformation of materials from OM_p to biomass (ΔG_{pd}, ΔG_{dc}, and ΔG_{cb}) are as follows:

$$OM_p \xrightarrow{-\Delta G_{pd}} OM_d \qquad \text{Breakdown or Dissolution}$$

$$OM_d \xrightarrow{-\Delta Gdc} CO_2 \qquad \text{Oxidation}$$

$$CO_2 + H_2O + NH_3 + HPO_4 \xrightarrow{+\Delta G_{cb}} \text{biomass} \qquad \text{Assimilation}$$

The bacteria may take part in either or both of the first two processes and, by definition, take part in the assimilation process. The associated free energies of the reactions may then be utilized by the bacteria for metabolic processes (growth, activity, etc.). The above equations, however, provide no information concerning the efficiency with which the bacteria can make use of the available energy. For use in computations of growth rates estimates of these efficiencies are needed as well as information on the standard free energies of formation, ΔG^o, of the OM_p, OM_d, bacterial biomass, and inorganic nutrients. Rate expressions for each of the processes are also required.

However, since the details of this approach have not been worked out, an empirical approach, which makes use of a rectangular hyperbolic function, has been used to describe bacterial growth as it is limited by energy availability alone. The concentration of total organic material (OM_T) is used as a measure of energy availability.

$$\hat{\mu}' = \hat{\mu} \left(\frac{OM_T}{K_s + OM_T}\right) \tag{16}$$

in which $\hat{\mu}'$ = growth rate limited by energy alone,

K_s = the concentration of OM_T that gives rise to a growth rate, $\hat{\mu}/2$,

$\hat{\mu}$ = maximum growth rate assuming no nutrient or energy limitations.

Given equation (9) for autotrophs and equation (16) for saprophages, equations may be formulated to describe growth rates for microbes in general as limited by inorganic nutrient concentration. To do so, equations must be

developed that take into consideration the various forms of the nutrient elements, carbon, nitrogen, and phosphorus. Organisms can utilize nutrients only in specific forms. A knowledge of these preferences is essential since environmental conditions and microbial populations exert a large effect on the distribution of nutrients among the various possible forms.

Some such information is currently available. From their observations that green algae grow more rapidly in acidic media, Emerson and Green[23] and Osterlind[24] concluded that these algae prefer dissolved CO_2 and/or carbonic acid to other forms of inorganic carbon. Keenan[25] reported that blue-green algae grew better at high pH's. Although he interpreted this as a direct pH dependence only, it may possibly be interpreted as a dependence on carbonate ion concentration. Little is said in the literature about the relative availability of ammonia and ammonium ion. However, judging from the pH values at which microbial growth optima occur, NH_4^+ is the more easily assimilated form. Based on similar information concerning the nutrient, phosphorus, the mono- and diprotonated forms of orthophosphate may be assumed to be preferred by microorganisms.

Organisms are known to utilize both nitrate and ammonia for growth. Some show a preference for nitrate and some for ammonia, although the reasons for these preferences are not always clear. Ammonia is believed to be, in general, more easily assimilated than nitrate because less energy is required for its conversion to amines.

When the specific chemical forms of the nutrients required for growth are known, their concentrations may be used in algebraic expressions relating growth to nutrient concentration. Many workers[4,26,27,28,29] have used an expression for the chemical nutrients that is comparable to the single factor of the Monod growth equation but is a product of several factors, one for each nutrient

$$\mu = \hat{\mu}' \prod_{i=1}^{n} \left(\frac{S_i}{K_s + S_i}\right) \tag{17}$$

in which n = total number of nutrients

S_i = concentration of nutrient, i

K_i = the concentration, S_i, that gives rise to that is one half of its maximum value (μ).

Another expression[21 27] uses the minimum of n quantities, $S_i/(K_i + S_i)$, $i = 1, 2, \ldots, n$, in place of the product of the n quantities in equation (17).

Droop[30] discussed another model incorporating Caperon's[31] suggestion that growth occurs by utilization of nutrients from internal pools. Droop argued for a linear relation between uptake rate and nutrient concentration in the cell, or cell quota (Q), in units of grams of nutrient per gram of biomass. Plots of uptake rate versus cell quota were linear, intersecting the Q-axis at a point, k_q (> 0), termed the "subsistence quota." At large values of cell quota (Q), he found that the asymptotic value of μ equals the slope of the plot of uptake versus cell quota. Based on this observation he derived the relation

$$\frac{\mu}{\mu_m'} = 1 - \frac{k_q}{Q}$$

in which μ_m' is the maximum growth rate resulting from internal nutrient concentration.

Three properties of the equation are important:

$\mu/\mu_m' \longrightarrow 1$ as Q becomes large,

$\mu \longrightarrow 0$ as $Q \longrightarrow k_q$,

$\mu = \frac{1}{2}\mu_m'$ when $Q = 2k_q$.

The first two properties are reasonable biologically, but the third is not. It seems unreasonable to expect that, in general, for a nutrient concentration of one half the half-saturation constant (k_q), growth will cease. Nevertheless, Droop has addressed the problem of describing algal growth with more care than previous workers, and his model or some variation may be found to be an improvement over previous ones for many uses. His formulation for algal growth in response to multiple nutrients is

$$\frac{\mu}{\mu_m'} = \prod_{i=1}^{n} \left(1 - \frac{k_{qi}}{Q_i}\right) \tag{18}$$

As Droop pointed out, this model predicts luxury uptake when nutrient concentration is high, but does not set an upper limit to the extent of this luxury uptake.

Equation (18) differs from equation (17) in several ways. It describes growth as occurring from internally stored nutrients. More significantly, it includes the

concept of a subsistence quota and, because it differs algebraically, some of the constants must be interpreted differently. However, in spite of these differences, results from the two equations do not differ greatly; equation (17), which requires fewer computations, is usually preferable.

For some green algae and for bacteria, both inorganic nutrients and small soluble organic molecules are used as substrates for growth. Thus some of the factors of equation (17) may include dissolved organic material. Algae, for example, are known to assimilate several sugars (including phosphorylated forms), fatty acids, and some amino acids[32], and to grow well using urea (apparently directly), amino acids, and amides (for some forms by extracellularly liberating ammonia)[33].

Energy Expense, Predation Rates, and Growth Rates of Small Biophagous Metazoa

Small metazoa (e.g., rotifers and crustacea) found in the plankton and periphyton are heterotrophic, and many feed upon living material. Because of these habits they are potentially important in the aquatic ecosystem, affecting nutrient cycles via their roles in the food web. Wiegert and Owen[22] termed such organisms "biophages" to distinguish them from saprophages, organisms that feed upon non-living organic material.

Submodels describing processes related to feeding and growth of biophages assume no age or size structures in the populations. Energy expense has usually been assumed to be constant, but the effects of the environment and of food availability on energy intake and expense may be important variables in the growth of motile forms.

Three types of models have been developed that may be used to describe the feeding and growth of small biophages. Lassiter and Hayne[34] presented a finite difference model, which considered that energy expense sets satiation level (maximum intake rate per unit time). The model predicted that when food was plentiful, the biophages were satiated and more energy was taken in than was expended. The difference was applied to growth of the population. The model is pedagogically useful, but it is difficult to use in differential equation models.

Other types of models relate growth directly to food intake without considering energy expense. Many of these models employ a single compartment to represent each trophic level[27,28,29]. These models are based on the assumption that a rectangular hyperbola adequately describes the feeding and growth rates of biophages. Lassiter[21] extended

these formulations to include multiple populations of biophages. The equation for growth rate, G_i, of the ith biophage population is given by

$$G_i = \hat{\mu}_i B_i \frac{\sum_{j=1}^{m} p_{ij} B_j}{K_i + \sum_{j=1}^{m} p_{ij} B_j} \tag{19}$$

in which $\hat{\mu}_i$ is maximal growth rate,

p_{ij} is a weighting constant defining the predation rate by the ith biophage on the jth prey type relative to the rate on any other prey type,

B_i is biomass of biophage,

B_j is biomass of prey,

K_i is the biomass of prey as modified by the weight, p, that result in half maximal biophage growth, and

m is the number of prey populations.

Feeding of small biophages results in losses to microbial populations. To compute the rate of death caused by predation on a microbial population, first the fraction of growth of a biophage population resulting from predation on a specific prey is needed. For biophage i feeding upon microbial organism k, the fraction is

$$F_{ki} = \frac{p_{ik} B_k}{\sum_{j=1}^{m} p_{ij} B_j} \tag{20}$$

Therefore the death rate to population k due to predation by r predators is

$$D = \sum_{i=1}^{r} \left(\frac{n_{ki}}{Y_i}\right) F_{ki} \, G_i \tag{21}$$

in which n_{ki} is a stoichiometric coefficient relating a unit of prey biomass to a unit of predator. The stoichiometric coefficient is useful when two or more nutrient cycles are

simultaneously of interest. It is a number relating the difference in empirical formulae of predator and prey, and it has the effect of setting the maximum yield. Using this approach the yield coefficient, Y_i, which usually represents the yield of predator per unit prey ingested, becomes an assimilation efficiency, a unitless number in the interval (0,1). For a discussion of predator-prey and other stoichiometry in ecosystem models (including yield), see Lassiter[21].

The third type of model[8] makes use of a submodel in which the constant, K, of the rectangular hyperbola is replaced by a term that is linearly related to biophage density. This expression has the effect of representing direct interference among predators competing for prey, whereas equation (19) incorporates only competition for the same prey population.

Neither equation (19) nor Bloomfield's submodel considers energy expense as a variable. However, either of the submodels could be rearranged to include energy budget equations if such could be developed. To do so, the yield coefficient in the submodels would have to be made a function of energy expense and intake.

Instead of modifying either equation, however, yet another equation was developed and used because of its mnemonic value. Redefining p_{ij} as the rate constant for predation of biophage i on prey j, the growth rate of biophage population i is given by

$$G_i = \frac{Y_i \, B_i \sum_j p_{ij} \, B_j}{n'_{ik} \, (K_i + \sum_j B_j)} \tag{22}$$

in which all other terms are as previously defined. In this submodel growth rate is a function of predation rate, assimilation efficiency (yield), and the stoichiometry relating the two. Maximal growth rate does not appear in the formulation. Feeding is represented in this function as the essential interaction, and growth as a result of the interaction. Since growth is a function of yield and yield is a function of an energy budget, growth is also a function of an energy budget.

Assuming equation (22) for growth of predators, rate of death caused by predation on population k is given by

$$D_k = \sum_{i=1}^{r} F_{ik} B_i \frac{\sum_j p_{ij} \, B_j}{K_i + \sum_j B_j} \tag{23}$$

in which all symbols are as previously defined.

In using these submodels in an ecosystem model, other couplings in the system must be considered. For example, at higher energy expense rates correspondingly greater input rates of CO_2 to the water from biophage metabolism must be accounted for. Patten[35] reasoned that a high degree of control exerted by higher trophic groups over lower is a significant and general feature of ecosystems. It was hypothesized from computer experimentation[21] that zooplankton activity in aquatic systems may markedly affect the behavior of every component. Thus effort spent in accurately computing rates of growth for consumer organisms may be rewarded by a large increase in the accuracy of resulting predictions of such quantities as producer standing crops and various aspects of material cycling.

Respiration, Death, and Excretion

Respiration is a general term for the metabolic functions required to maintain the physiological integrity of organisms. Its uses in ecosystem modeling are manifold: mass balances for O_2 and CO_2, terms in net growth equations, and energy balance terms. A functional module for respiration, then, will be a very much used term. It may be a very simple function such as might be used for microbial respiration, or it may be rather complex such as the several terms relating to respiration in the energy budget[34]. If respiration is assumed to be a function of temperature alone, equation (13) may be used. For respiration the optimum temperature, T_m, and the upper limiting temperature, T_L, usually are fairly close together, resulting in a rapid decline in rate as the temperature increases for T_m to T_L.

Two classes of anabolic processes appear to be operative in organisms, viz., those processes involved in creating new structure, which have their temperature optima well below the limiting temperature, and those processes that function in repair, which operate more effectively with increasing physiological stress. The latter type are respiratory processes and reach a maximum only when heat denatures the proteins involved, the process occurring at T_L.

Death to organisms may result from several causes. Predation has already been discussed and equations have been presented to describe it (equations 21 and 23). Temperature may also exert lethal affects. Death rate due to temperature may be described by the following expression:

$$D_T = \begin{cases} -a \ln k/k_m & T \geq T_m \\ 0 & T < T_m \end{cases} \qquad (24)$$

in which D is the specific death rate due to excessive temperature, a is a scaling constant, and k is from equation (13).

Death to natural populations also results from several unspecifiable causes, the probability of which is assumed to remain constant for each of the organisms. Therefore, the specific death rate from causes other than excessive temperature or predation is simply a constant in the differential equation.

Excretion represents yet another mechanism by which biological populations may lose biomass. Algae are known to excrete small organic compounds[36] the physiological mechanism of which, however, is unclear. The specific rate of excretion is therefore assumed to be constant.

For consumers, excretion may result from several causes. Metabolic products resulting from catabolic processes may be excreted, which argues for an excretion rate proportional to metabolic rate. The excretion of metabolic products, then, may be represented as proportional to the temperature dependent respiration rate.

Another process that necessarily results in excretion by consumers is the imperfect matching of the composition of food biomass and consumer biomass. This is a problem in predator-prey stoichiometry, and was discussed in detail by Lassiter[21]. A stoichiometric coefficient is formed for the units of food consumed per comparable unit of consumer formed. This coefficient varies depending upon the composition of the food. It is used to compute another coefficient, n, for excretion of an element by the consumer. The excretion rate, E_i, for population i is then simply

$$E_i = nG_i.$$

Inhibition

One other submodel has proved beneficial, viz., an expression for the inhibition of biological processes by the presence of some specific chemical species. This may be actual inhibition, for example, inhibition of denitrification by the presence of oxygen, or it could reflect a preference, such as inhibition of uptake of NO_3^- by presence of "preferred" NH_3 by microorganisms.

The change in the rate coefficient, k, of the inhibited process with respect to the inhibiting substance is assumed to be proportional both to the value of the coefficient and to the concentration, x, of the inhibiting substance.

These assumptions may be rationalized on the following bases: first the rate coefficient must remain in the interval $(0, k_m)$ and therefore a change in response to an external stimulus must be a function of the rate itself; and second, the change in k with x for a particular process is dependent upon the particular value of x, subject to change by physiological adaptation. These assumptions may be stated as

$$\frac{\partial k}{\partial x} = -akx \tag{25}$$

which, upon integration gives

$$k = k_m e^{-ax^2} \tag{26}$$

in which a is a scaling coefficient and the other symbols are as previously defined.

When two or more substances independently inhibit a process, equation (2) can be extended to

$$k = k_m e^{-(\sum_{i=1}^{n} a_i x_i^2)} \tag{27}$$

in which there are n inhibiting substances.

By suitable choice of constants, a_i, the inhibition function may be made to blend processes smoothly or to switch a process on or off within a very small range of concentration of the inhibitor.

SECTION V

A PRELIMINARY MODEL FOR THE NITROGEN CYCLE

In constructing a model for a system or for one of its subsystems, some logical sequence of steps should be followed so that errors, repetition, and the time required for the task may be minimized. A model for the nitrogen cycle, as a subsystem of an aquatic ecosystem, was developed following the procedure discussed in Section III, The Modeling Process. Because this model is viewed as a preliminary model to be revised when incorporated into a more comprehensive ecosystem model, the modeling process will be used again when the revision occurs and other submodels are included. Some of the submodels developed in the previous section were used as modules in building the larger, nitrogen cycle model.

PROBLEM DEFINITION

Many ecosystem models have been constructed using first-order or other approximations to only portions of the nitrogen cycle[4,21,26,27,28,29]. None have attempted a mechanistic description of the complete cycle. Textbook and other general descriptions[37,38,39,40] indicate that compensatory aspects of the nitrogen cycle may be important in producing a realistic model. That is, depletion and replenishment should be represented to accurately model nitrogen dynamics. A nitrogen model was developed to take into consideration the compensatory aspects of the cycle more completely and to examine the benefits derived from the more complete representation. The model was to be constructed to permit examination of the influence of pollutants on nitrogen transformations, e.g., the influence of mercury on nitrification rates.

The minimal set of system variables chosen included ammonia, nitrite, nitrate, and organic nitrogen.

SYSTEM DIAGRAM

System diagrams representing the four variables helped to define the couplings, influences, and other processes that must be included in the model. Figures 9 and 10 represent a final version of the diagrams used in the model development.

Ammonia is a product of the decomposition of organic nitrogen. The rate of the decomposition process is a function of oxygen concentration, as are most other processes of the nitrogen cycle. Therefore oxygen is

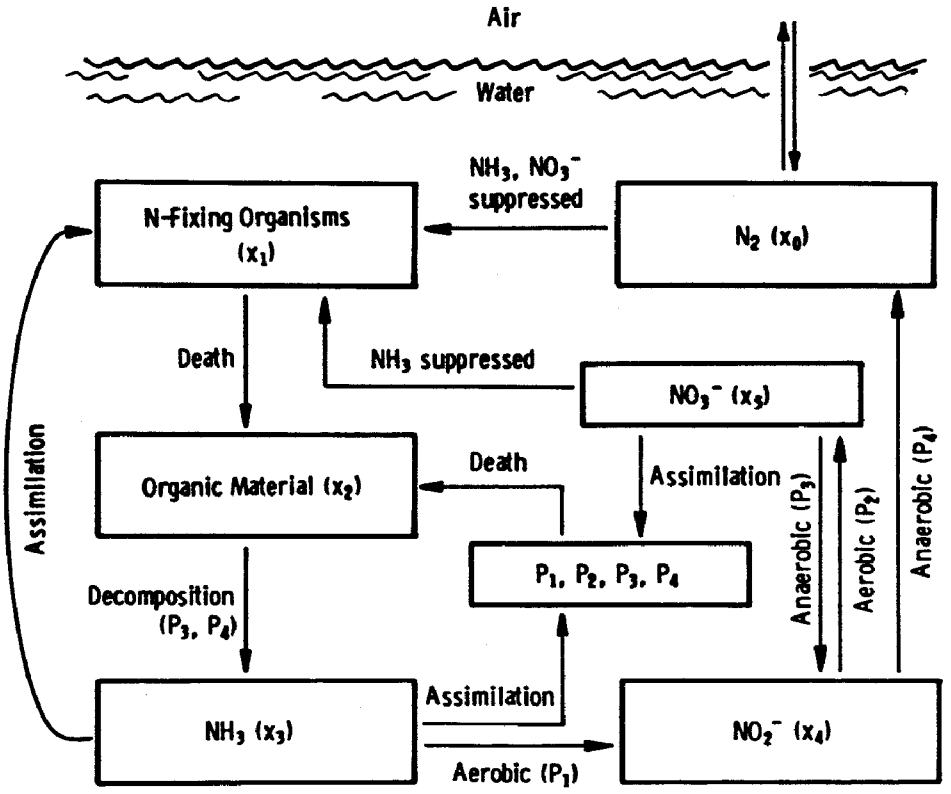

Figure 9. Diagram of system components and transfers for the nitrogen cycle as depicted by equations (28) through (32).

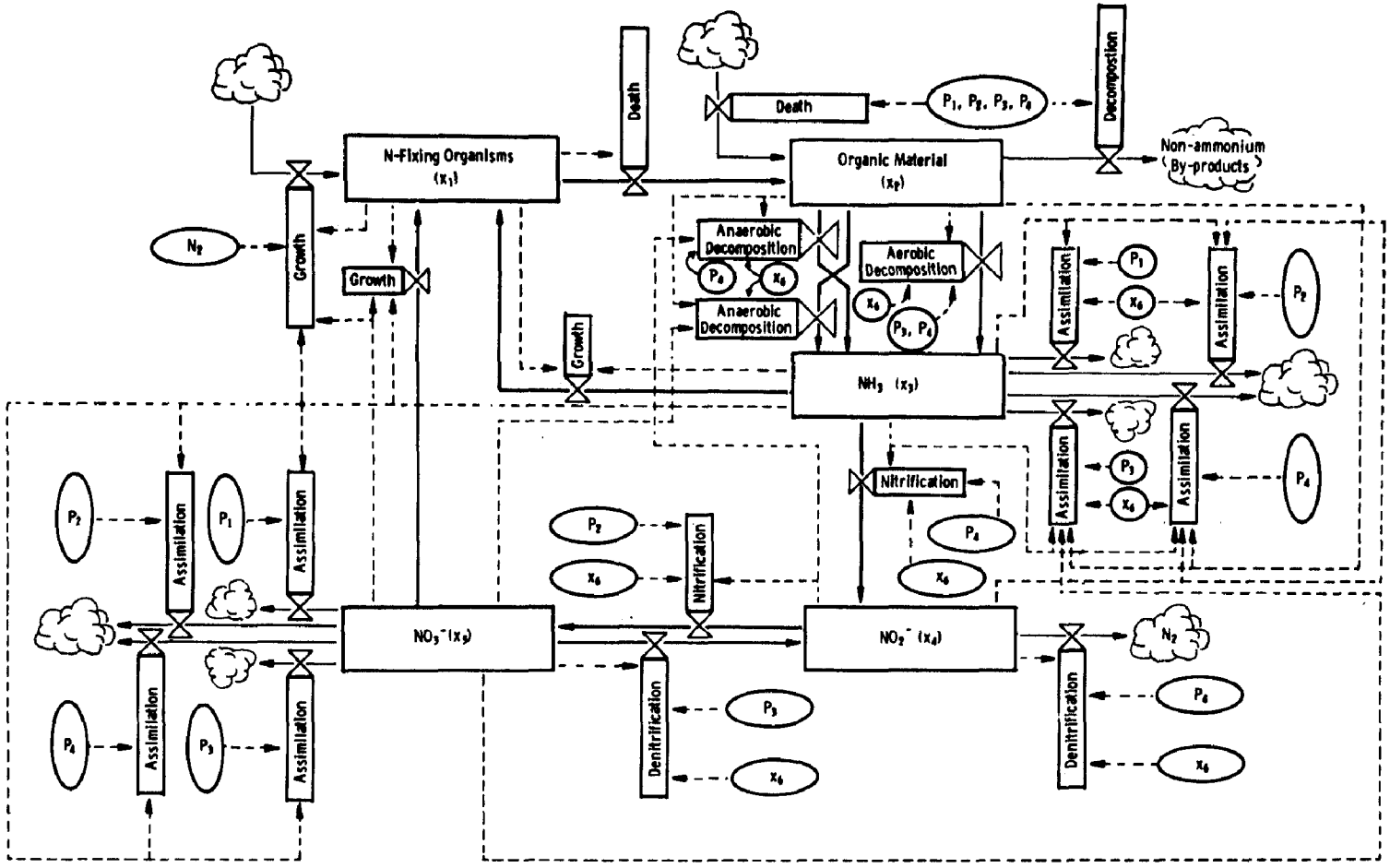

Figure 10. Forrester diagram of the nitrogen cycle (equations 28 through 32) showing more explicitly the processes and points of influence of the components.

required either as a system input or as a system variable. For this model, it proved more useful to use it as an input (forcing) function.

Organic nitrogen is produced by four processes: microbial assimilation of ammonia, nitrite, and nitrate, and fixation of elemental nitrogen. Because nitrite occurs at very low concentrations, its assimilation could be ignored for the present purposes. Both nitrate and ammonia suppress N-fixation, although ammonia is the more effective suppressant[36]. To keep the diagram (and later the mathematical model) as simple as possible, only one type of organism was represented by a dynamic variable. (For other microorganisms, fixed population sizes were assumed.) This organism was assumed to fix elemental nitrogen if neither nitrate nor ammonia was plentiful and thus to replenish the nitrogen in the system when it became depleted. Deaths from this population and from the fixed size populations contributed to the organic nitrogen pool.

Ammonia disappears by two processes: assimilation (producing organic nitrogen as noted previously), and nitrification. Nitrification was assumed to proceed in two steps: (1) $NH_3 \longrightarrow NO_2^-$, and (2) $NO_2^- \longrightarrow NO_3^-$. Both use oxygen as the oxidizing agent.

Decomposition of organic nitrogen can occur both aerobically and anaerobically. Anaerobic decomposition may proceed by several mechanisms. For initial simplicity, decomposition was assumed to be carried out by two fixed-size populations of microorganisms. Both were assumed to be facultative anaerobes, switching their metabolism from aerobic to anaerobic according to prevailing conditions. One was assumed capable of using nitrite and the other capable of using nitrate as oxidizing agents. Other possible competing anaerobic processes were ignored.

Nitrite is produced when facultative anaerobes utilize NO_3^- as the oxidizing agent in the decomposition of organic matter (denitrification), and when they oxidize NH_3 (nitrification). Denitrification is said to be inversely related to redox potential[41]. However, according to Hardy[42], the denitrifying enzymes are sensitive to oxygen concentration; above 0.2 mg O_2/l, the enzymes are repressed. At low oxygen concentrations, which usually occur at low redox potentials, the denitrifying enzymes are de-repressed and denitrification can proceed.

Nitrate arises by nitrification of NO_2^- and disappears by assimilation into microbial biomass and by denitrification.

Finally, nitrogen is gained by fixation of N_2, as discussed previously, and is lost as N_2, the end-product of

denitrification. Thus the cycle is closed in the causal sense. It is open, however, inasmuch as N_2 is for all practical purposes an infinite source-sink reservoir.

PROCESS MECHANISMS

For this model simple constructs were used to express the essential aspects of the system. For example, the customary hyperbolic function (equation 17) was not used in the description of growth rates, but the inhibition function (equation 27) was used extensively. The equations were coupled such that exchange of gaseous nitrogen was the only mechanism for loss or gain for the system.

The nitrogen cycle in nature requires both oxygen-replete and oxygen-depleted environments for all processes to occur. All processes described in this single model were assumed to proceed concurrently, except when inhibition or resources limited rates to near zero. For example, oxygen was used to switch the nitrification and denitrification processes on and off, simulating aerobic and anaerobic environments.

Five dynamic variables were used in the model:

x_1 = organisms capable of assimilating NH_3 and NO_2^-, and of fixing N_2; expressed as concentration,

x_2 = concentration of organic material (containing N in the same fixed proportion as x_1),

x_3 = NH_3 as [N],

x_4 = NO_2^- as [N], and

x_5 = NO_3^- as [N].

Oxygen was made time varying and was labeled x_6. Four fixed-size populations were included (P_1, P_2, P_3, and P_4). Nitrification steps ($NH_3 \longrightarrow NO_2^-$) and ($NO_2^- \longrightarrow NO_3^-$) were mediated by P_1 and P_2, respectively. Denitrification steps ($NO_3^- \longrightarrow NO_2^-$) and ($NO_2^- \longrightarrow N_2$) were mediated by P_3 and P_4, respectively. Elemental nitrogen was denoted by x_0, and was assumed to be present at saturation concentrations.

Inhibition functions of the form of equations (26) and (27) are denoted generically (each may differ in coefficients) by $I(x_i)$ or $I(x_i, x_j)$ in the following description of the interactions and construction of equations. Also stoichiometric coefficients are generically represented as S. The rate coefficients for the various processes are symbolized by k's with subscripts. The subscripts have no value for identifying the process to

which they belong other than to allow one to distinguish whether terms of different equations refer to the same process.

The equation for x_1 consists of terms for assimilation and death:

$$\frac{dx_1}{dt} = [k_{00}x_0\ I(x_3,x_5) + k_{01}x_5\ I(x_3) + k_{02}x_3 - k_1]x_1 \qquad (28)$$

Note that N-fixation (first term) is inhibited by both NH_3 (x_3) and NO_3^- (x_5), while NO_3^- assimilation (second term) is inhibited by NH_3 only.

Organic nitrogen was represented as a fixed portion of organic material (10 moles of N atoms per mole of organic material). The chemical compositions of P_1, P_2, P_3, P_4, and x_1 were assumed to be identical. The equation for the appearance and disappearance of x_2 was constructed:

$$\begin{aligned}\frac{dx_2}{dt} = {} & k_1x_1 + k_2P_1 + k_3P_2 + k_4P_3 + k_5P_4 \\ & - (k_6P_3 + k_7P_4)x_2x_6 \\ & - k_{13}\ I(x_6)\ P_3x_2x_5 \\ & - k_{15}\ I(x_6)\ P_4x_2x_4\end{aligned} \qquad (29)$$

in which the positive terms are inputs from deaths of the indicated populations, the first negative term represents aerobic organic decomposition, and the last two negative terms, anaerobic decomposition.

Both nitrate and ammonia are readily assimilated by most microorganisms, but ammonia is the more frequently preferred form. Aerobic decomposition, denitrification, and nitrification are all microbially mediated processes from which the organisms obtain energy to assimilate biomass. Thus with each of these processes there is accompanying assimilation of ammonia or nitrate. Assimilation terms for both ammonia and nitrate are represented as proportional to the product of the energy yielding process and the concentration of NH_3 (or NO_3^-). The equations for ammonia (x_3) and nitrate (x_5) are given below (together because of similarity), followed by the equation for nitrite.

For ammonia:

$$\frac{dx_3}{dt} = S\ [k_{13}\ I(x_6)\ P_3x_2x_5 \qquad (30.1)$$

$$+\ k_{15}\ I(x_6)\ P_4x_2x_4 \qquad (30.2)$$

$$+\ (k_6P_3 + k_7P_4)x_2x_6] \qquad (30.3)$$

$$-\ k_{02}x_1x_3 \qquad (30.4)$$

$$-\ [k_8k_{12}P_1x_3x_6 \qquad (30.5)$$

$$+\ k_9k_{14}P_2x_4x_6 \qquad (30.6)$$

$$+\ k_{10}k_{13}\ I(x_6)P_3x_2x_5 \qquad (30.7)$$

$$+\ k_{11}k_{15}\ I(x_6)P_4x_2x_4]x_3 \qquad (30.8)$$

$$-\ k_{12}P_1x_3x_6 \qquad (30.9)$$

The terms in the NH_3 equation are

30.1 anaerobic decomposition using NO_3^- as the oxidizing agent,

30.2 anaerobic decomposition using NO_2^- as the oxidizing agent,

30.3 aerobic decomposition,

30.4 assimilation by x_1,

30.5 assimilation by P_1 accompanying the net reaction, $NH_3 \longrightarrow NO_2^-$,

30.6 assimilation by P_2 accompanying the net reaction, $NO_2^- \longrightarrow NO_3^-$,

30.7 assimilation by P_3 accompanying decomposition of organic material using NO_3^-,

30.8 assimilation by P_4 accompanying decomposition of organic material using NO_2^-, and

30.9 direct nitrification, $NH_3 \longrightarrow NO_2^-$.

For nitrate:

$$\frac{dx_5}{dt} = k_{14}P_2x_4x_6 \tag{31.1}$$

$$- [S\ k_{13}\ I(x_6)P_3x_2 \tag{31.2}$$

$$+ x_1k_{01}I(x_3) \tag{31.3}$$

$$+ k_{81}\ I(x_3)k_{12}P_1x_3x_6 \tag{31.4}$$

$$+ k_{91}\ I(x_3)k_{14}P_2x_4x_6 \tag{31.5}$$

$$+ k_{101}\ I(x_3)k_{13}P_3x_2x_5 \tag{31.6}$$

$$+ k_{111}\ I(x_3)k_{15}\ I(x_6)P_4x_2x_4]x_5 \tag{31.7}$$

The terms in the NO_3^- equation are

31.1 nitrification, $NO_2^- \longrightarrow NO_3^-$,

31.2 denitrification, $NO_3^- \longrightarrow NO_2^-$,

31.3 assimilation by X_1,

31.4 assimilation by P_1 accompanying the net reaction, $NH_3 \longrightarrow NO_2^-$,

31.5 assimilation by P_2 accompanying the net reaction, $NO_2^- \longrightarrow NO_3^-$,

31.6 assimilation by P_3 accompanying decomposition of organic material using NO_3^-,

31.7 assimilation by P_4 accompanying decomposition of organic material using NO_2.

The NH_3 and the NO_3^- equations are similar in some respects and different in others. Three modes of decomposition are direct sources for NH_3 (in the real world there are more than three), and only one process, nitrification, results in NO_3^-. All the loss terms are similar, except for the inhibition of NO_3^- loss by the presence of ammonia (in the real world the difference is not so distinct).

The equation for nitrite is given by

$$\frac{dx_4}{dt} = k_{12}P_1x_3x_6 + S\,k_{13}\,I(x_6)P_3x_2x_5 - S\,k_{14}P_2x_4x_6 - S\,k_{15}\,I(x_6)P_4x_2x_4 \tag{32}$$

The nitrite equation includes no assimilation term. The first term is input by nitrification, $NH_3 \longrightarrow NO_2^-$, and the second is input by denitrification, $NO_3^- \longrightarrow NO_2^-$. The third term represents loss via nitrification, $NO_2^- \longrightarrow NO_3^-$, and the fourth, for denitrification, $NO_2^- \longrightarrow N_2$.

These equations, even without hyperbolic or other descriptive factors, are uncomfortably complex. The complexity, however, is necessary if the model is to include the couplings and influences depicted in Figures 9 and 10. The numerous influences upon most of the rates give rise to long terms in the equation; the highly coupled nature of the cycle gives rise to many terms in each equation.

ESTIMATION OF PARAMETERS

Ideally values for parameters for such a model would be determined from data from applicable experiments. All of the parameters however, were merely estimated. Using a model such as this in which each term contains several factors, each of which is constrained to non-negative values, it becomes very clear that parameter estimates are strong functions of the form of the model. Initial parameter estimates ranged from 0.0012 for the rate constants for assimilation of ammonia and nitrate by denitrifying organisms to 1.1×10^{12} for the rate constant for decomposition of organic material by those same organisms. To one used to thinking in terms of first-order rate constants, these values (especially the latter) may seem absurd. Had the factors appeared as rectangular hyperbolae, so that each factor was unitless and constrained to the interval (0, 1), the parameter estimates would have approximated first-order rate constants.

ANALYSIS OF PRELIMINARY RESULTS

The results indicate that this model or a similar one should be a part of a larger ecosystem model if part of the purpose of the larger model is to describe the transient behavior of dissolved chemicals. Steady state results for the four chemical components for both aerobic and anaerobic conditions are shown in Figure 11. Output from the model indicated that the net rates of change for some processes were of the right order of magnitude to be included in a larger model. Also, the behavior of the components was shown to be interdependent so that each component is affected by every other component either directly or indirectly.

The parameter estimates may have been badly in error. Such a possibility is suggested by the relatively high steady state NO_2^- values under aerobic conditions and the relative stability of NH_3 under a change from aerobic to anaerobic conditions. The high aerobic NO_2^- values are partially explainable by the failure of the model to contain assimilation terms. The high turnover rate of NH_3 resulting from inputs and outputs under both aerobic and anaerobic conditions may help explain its stability.

The whole cycle may be considered to be comprised of the anaerobic (denitrification) subsystem, and the aerobic (nitrification) subsystem with N-fixation occurring in both. For denitrification to occur, nitrification must already have occurred. Tusneem and Patrick[43] showed that for continuously flooded soils denitrification rate was dependent upon the size of the aerobic layer in which nitrification occurred. This model operates in the same manner, *i.e.*, a switch to anaerobic conditions obviously results in little denitrification if little NO_3^- has been formed by nitrification.

Further work is needed to improve the model. Nitrite assimilation should be added, and the whole model should be divided into aerobic and anaerobic coupled subsystems. Improved parameter estimates should be made. Subsequently, it will be incorporated into an ecosystem model coupled to chemical equilibria and tested with dynamically varying organism and dissolved O_2 concentrations. Coupled with models for pollutants shown to affect the metabolism of one or more of the types of organisms active in the cycle, perhaps it may yield estimates of system impact of the pollutant and shorten the investigative process.

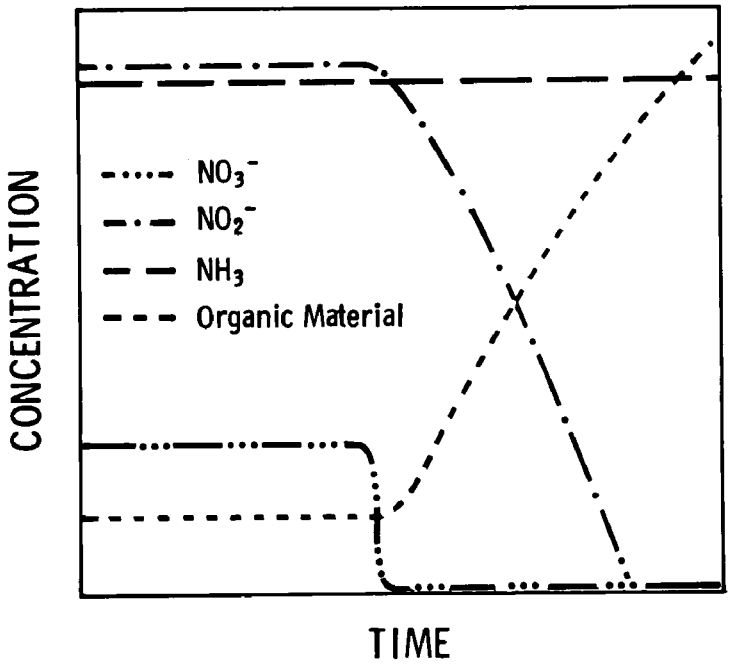

Figure 11. Relative steady state concentrations of four chemical components of the nitrogen cycle model. Results show a change from aerobic to anaerobic conditions.

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16. ABSTRACT

To provide capability to model aquatic ecosystems or their subsystems as needed for particular research goals, a modeling strategy was developed. Submodels of several processes common to aquatic ecosystems were developed or adapted from previously existing ones. Included are submodels for photosynthesis as a function of light and depth, biological growth rates as a function of temperature, dynamic chemical equilibrium, feeding and growth, and various types of losses to biological populations. These submodels may be used as modules in the construction of models of subsystems or ecosystems. A preliminary model for the nitrogen cycle subsystem was developed using the modeling strategy and applicable submodels.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Computerized Simulation Photosynthesis Phytoplankton; Zooplankton Water Chemistry Nitrogen cycle Limnology	Predator-prey models Inhibition model Microbial Growth Rate Algal Growth Rate Aquatic Ecosystem Model Temperature Related Growth	06/06 06/13 08/08

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