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SUBJECT: Transmittal of ORD Final Report "Prediction of Ecological Effects of Toxic Chemicals: Overall Strategy and Theoretical Basis for the Ecosystem Model"

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The attached ORD research report (EPA-660/3-83-084) which was recently released is being transmitted to you for your use. The report responds to the Agency's need for predictive models of toxic chemical effects in natural waters.

The objective of this research was to develop the rationale for a prognostic model for ecological effects of toxic chemicals. Included were efforts to more clearly define the scope of "ecological effects," to define the level of resolution needed to permit application of existing toxicological measures, to analyze available toxicity data statistically, and to initiate development of a working model.

In this research project, performed under EPA's Innovative Research Program, a strategy was developed for modeling ecosystems to permit assessment of effects of toxic chemicals on element cycling and other cosystem processes. Progress also was made in defining ecological effects, establishing model resolution requirements, and providing stat-Tstical analysis of data on the LC50 toxicity measure. The research provides a basis for continuing work toward a prognostic evaluation model for new chemicals or those without extensive field data.

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Prediction of Ecological Effects of Toxic Chemicals: Overall Strategy and Theoretical Basis for the Ecosystem Model

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The information in this document has been funded wholly or in part by the United States Environmental Protection Agency under Cooperative Agreement No. CR808629 with the University of Georgia. It has been subject to the Agency's peer and administrative review, and it has been approved for publication as an EPA document.

FOREWORD

Environmental protection efforts are increasingly directed toward preventing adverse health and ecological effects associated with specific compounds of natural or human origin. As part of this laboratory's research on the occurrence, movement, transformation, impact, and control of environmental contaminants, the Environmental Systems Branch studies complexes of environmental processes that control the transport, transformation, degradation, fate, and impact of pollutants or other materials in soil and water and develops models for assessing exposures to chemical contaminants.

Concern about adverse environmental effects of synthetic organic compounds has increased the need for techniques to predict the ecological effects of chemicals entering the environment as a result of the manufacture, use, and disposal of commercial products. This research is directed toward a new approach to predicting the probable effects of toxic chemicals expressly for environmental assessment. The research was done under one of the USEPA's Innovative Research Projects. The research is continuing toward providing the capacity to assess the ecological effects of chemicals particularly on element cycling processes. Upon completion it is anticipated that it will comprise one of the components in a risk analysis system.

William T. Donaldson
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PREFACE

It is very difficult conceptually to design a means by which effects of toxic chemicals in natural waters can be predicted. Part of the difficulty lies in identifying exactly what those effects are. Determining the scale of the effect of interest is a particularly difficult aspect of the identification problem. In particular, it must be determined whether the effect of interest is expressed at the chemical, biochemical, physiological, individual, population, community or even larger scale. Most experimental studies are carried out at the finer scales of resolution, whereas most of our ultimate interest with respect to environmental risk is at the coarser and more integrated scales. Experimental studies have been done at the finer scales partly because they are the scales that can be readily handled experimentally, but also, I believe, because there is an implicit assumption that there are comprehensible connections between behavior at the finer scales and that at the coarser. That is, it seems to me that there is a general expectation that inferences can be drawn about the ecological scale behavior and results obtained at the finer scales of resolution. The aim of this study is to provide a mechanism for making such inferences. Specifically, my aim is to predict behavior at the ecological level of organization based upon considerations at the lower levels. This report details my efforts toward that end.

The project began as a result of a proposal to EPA's Innovative Research Program. Under this program I carried out two years of research at the University of Georgia in the Institute of Ecology. The subject partitioned naturally into two major subareas, one on the specific representation of the aquatic ecosystem and the other on the specific representation of the direct effects of toxicants. Approximately equal time was spent on the two subprojects. The subproject on representing the direct effects did not progress as well, however, as the subproject on ecosystem representation. For this reason the direct effects subproject is not reported in detail. Only the rationale for interfacing the representation of direct effects with the ecosystem representation is discussed.

This report is intended to convey two major sets of ideas and to give the specifics of one of them. The first idea is the overall approach and its rationale. The second is the idea on which the ecosystem representation is based. This idea is that ecosystem processes can be described functionally as material and energy transduction, and that the embodiment of these functions by discrete species is an essential feature of ecosystems that must be represented if ecosystem-like behavior is to be achieved by the model. Relative stability of processes in the presence of fluctuations of species carrying them out is an example. Specific equations describing most of the functional ecological processes occupy most of the volume of the report. The level of detail used in the presentation is intended to indicate the level

of resolution to be used and to document the specifics of the ecosystem model as it will be translated into computer code.

The overall goal of developing the capability to predict the ecological effects of toxic chemicals has not yet been achieved. On the contrary the difficulty and magnitude of the project are realized to be greater than was at first appreciated. Nevertheless, the potential to achieve that goal still appears to be good. Work has begun toward a computer code for the multi-species ecosystem model, and work is continuing on a sound representation of direct effects to include the simultaneous action of multiple chemicals. One major area of the ecosystem representation that still needs further work is that of fermentation, probably of great importance in the cycling of elements.

The opportunity to work for two years, relatively unencumbered, on this project is greatly appreciated. I extend thanks to the numerous individuals associated with the U. S. Environmental Protection Agency's Innovative Research Program and the Athens Environmental Research Laboratory who made it possible for me to do this research. Among those individuals, I am especially appreciative of the efforts of the project officer, Dr. Morris Levin, of the support of the former laboratory director, Dr. David Duttweiler, and of the innovative and untiring effort of Ms. Connie Shoemaker to work out the institutional arrangements between the EPA and the University of Georgia. I thank Ronnie Moon and Bruce Bartell for drafting the figures.

The Institute of Ecology at the University of Georgia graciously made their facilities available to me for the term of the project. Dr. James Cooley, Director of that institute served as the official principal investigator for the project and was helpful in numerous ways. To him and other individuals at The Institute I am appreciative. Of all individuals who contributed ideas and constructive criticism, no one was more helpful than Mr. Robert Hermann, graduate student in ecology. Providing continuity, coherence, and logical completeness to the theoretical basis for this modeling approach was the most important, difficult, and time consuming part of this project. In these efforts Bob Hermann was of inestimable help with his willing assistance and input through many protracted, and undoubtedly sometimes disjointed, discussions. Discussions of these and many related ideas in a weekly seminar led by Dr. Bernard Patten and myself provided continual stimulation and difficult to assess, but certainly positive, benefit.

It is traditional for authors to make a statement of explicit assumption of errors of omission, logic, or other sorts. Such a statement is more necessary here than usual, because of the stage of the research on which I report. It is probable that there are errors, and, in spite of all the invaluable assistance generously given me, the errors are definitely my own.

Finally, this report officially is the final report at the end of

the term of the Innovative Research project, but I intend that it be considered to function more as a progress report. My admittedly biased assessment of the potential for results of this project when successfully completed are that it is of a high magnitude. It is my hope and intent to add to this report on the theoretical basis for the ecosystem model, additional reports on the basis for the ecotoxicology model, on the design, implementation, and initial results from the working computer model, and on results of experiments to test predictions of the model.

ABSTRACT

A strategy for predicting the ecological effects of toxic chemicals in aquatic systems is developed. The strategy for obtaining the predictions is to carry out a process of several steps. The ecosystem is obtained first by specifying characteristics of the abiotic and biotic systems. The biotic system is initially represented by a large set of state variables representing potential species that initially exist in the environment. The operating ecosystem is obtained by selecting via computer simulation the smaller set of state variables that persist for an arbitrary period. The resulting system is a synthetic system. Any one synthetic system represents real systems only in a general way. Monte Carlo techniques are to be used to obtain a distribution of synthetic systems that persist for the arbitrary period in the given environment. Characteristics of a real system that could occupy a real environment similar to the one described are expected to be included in the distribution. Ecological effects are obtained by comparing computer simulations that differ only in the presence or absence of a toxic chemical along with its direct effects.

The ecosystem is to be described in the computer simulation as a set of differential equations representing the biotic and chemical species. Processes that occur in ecosystems are described fundamentally as energy transductions. Organisms are represented as reaction systems carrying out kinetically hindered redox reactions and using part of the released energy for metabolism, activity, and growth. Elements are cycled between their oxidized and reduced states via these biotically catalyzed redox reactions. The fundamental distinction between autotrophy and heterotrophy is recognized and their complementary roles in element cycles are represented. Distinction between the modes of ecological coupling of micro- and macroorganisms is recognized.

Mathematical models of growth of autotrophs and heterotrophs are assimilated or developed. The level of resolution used in these models is selected to permit coupling of toxic effects by mode of action of the toxicant. It is argued that the relevance of the synthetic approach to modeling the ecological effects of toxic chemicals depends upon the fidelity with which the model processes represent real processes; not on an inherent limitation of the approach.

This report covers the period from November 1980 to June 1983, and the work reported was completed as of February 1983.

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INTRODUCTION

When analyzing the risks associated with the presence of toxic chemicals in the environment, one can be concerned with a variety of potential effects. Effects that are manifested not as a result of direct toxicity but as alterations of the interrelationships among organisms and with their chemical and physical environment are most difficult to evaluate. Many possible effects of this sort are recognized. Alterations in element cycles, for example, are one set of such effects worth considering for their potential to change environmental levels of natural chemicals. An ecosystem model representing the processes important in element cycling, if based on fundamental theory, in principle could be used to predict effects on element cycling. There is a practical difficulty, however, in basing an operating model on fundamental considerations. Element cycle transformation rates are rather stable, relative to fluctuations typical of individual populations. It is nearly compelling to visualize that this stability arises from the presence of populations of several species able to carry out a single process. In this view loss or diminution of a population is followed by compensating increases in one or more others, so that the function (element cycle transformation) is carried out rather smoothly even in the presence of extreme fluctuations of the individual populations involved. The difficulty lies in finding an appropriate representation for a system, so that the model will exhibit whatever functional stability that results from compensation by competing species. In addition the representation must permit the coupling of toxicological and other effects to system components (species, chemicals, chemical pools, etc.) in such a manner that destabilization of system functions will be predicted when appropriate. No simple solution to this problem is apparent. My approach is to describe the ecosystem using a system of differential equations for which the associated state variables represent population densities or chemical concentrations. System functions are fluxes of materials and energy and are represented by terms that couple these equations. Several equations representing biotic species will each contain a term representing a single function so that both compensation and toxicological effects can be represented. Such a model will be very large, potentially with a few hundred state variables. There are associated methodological difficulties, and these have not been ignored. For this report, however, I shall not discuss them, so that I may focus on the model and its theoretical derivation. Because of my intent for the model to be comprised, in part, of the explicit representation of many species, all derivations of the descriptions of interactions will be made with the assumption of the existence of an arbitrary number of species in the system.

One potential difficulty in using a model comprised of many state variables to represent a community comprised of a large number of species is design of the mechanism for achieving the coupling structure for trophic interactions. The approach that makes the least demand on the underlying theory is to use a set of

predation rates assigned to species pairs (the per capita rate at which one species feeds on another). I have chosen to use a different approach, however, in which feeding rates are calculated from morphological and behavioral characteristics and swimming velocities of predator and prey. It is presumed that these characteristics could be determined for individual species. The rationale is that any quantity that can be measured for individuals of a species is much more accessible than are quantities requiring observation of the interactions of individuals of two or more species. The latter kind of measurements will seldom be available.

THE NATURE OF ELEMENT CYCLES AND IMPORTANCE OF CONSIDERING THEIR RESPONSE TO TOXICANTS

All processes occur as changes from disequilibrium toward equilibrium conditions. Biotic processes predominantly occur as a result of redox disequilibria. Plant photosynthesis creates the highest degree of disequilibrium by producing both reduced carbon and the strong oxidant, molecular oxygen. Aerobic respiration is the converse process. In this same sense anaerobic respiration, in which oxidants other than oxygen are reduced, and chemosynthesis are converse processes. Chemosynthesis is driven by energy released upon oxidation of reduced forms of N, S, and C. Because light drives photosynthesis and is available in aerobic environments, photosynthesis and its converse process, aerobic respiration, can proceed in the same environments. Respiration using oxidized forms of N, S, and C, however, proceeds only in anaerobic environments, whereas the converse processes (chemosynthetic processes utilizing the same elements) proceed only in aerobic environments. Thus for these components of element cycles, reduced forms of elements must be transported into aerobic environments for chemosynthesis and accompanying oxidation of the elements to occur. Completion of element cycles does not necessarily depend on transport between environments, however. Reduction of oxidized forms also occurs during biosynthesis regardless of the environment. Most organisms that live in aerobic environments can incorporate amino and thiol groups into biomass by obtaining oxidized forms of N and S from the environment and reducing them internally. This is assimilatory reduction (to distinguish from dissimilatory reduction, the comparable term corresponding to respiration using electron acceptors other than oxygen). Upon death and decomposition in aerobic environments, these reduced forms are either assimilated directly or oxidized via chemosynthesis. By these mechanisms element cycles are complete in aerobic environments.

The relative importance of assimilatory and dissimilatory pathways in maintaining local and global pool sizes of elemental forms is not clear, nor is the importance of the role of abiotic processes or boundary conditions imposed by geological and meteorological factors relative to biotic factors. If, in principle, these factors are included, however, it is fair to

say that element cycling is responsible for pool sizes of geochemicals. These include the atmospheric gases, the composition of the oceans, and the earth's soils. The remarkable stability of these characteristics over geological time scales (1) probably is indicative of the robustness of the component processes (perhaps due largely to functional compensation arising from species diversity). No comparative analysis of the role of biotic versus abiotic processes in element cycling has been made, but the number and importance of processes known to be carried out by organisms leaves no doubt that the characteristics of the earth depend on the continuation of biotic processes at about the level that they are presently occurring. Large scale introduction of new xenobiotic chemicals into the biosphere is a practice that has been occurring for only a short time. Whether the robustness that apparently has been exhibited over geological time will continue in the presence of these chemicals is not known. It is prudent, therefore, to make the effort to consider potential changes in element cycling, to make it possible to identify conditions that might lead to serious results, and, equally importantly, to provide an estimate of the probability that the change will occur.

BASIC ASPECTS OF A MODEL FOR PREDICTING ECOSYSTEM EFFECTS

The importance of the ecosystem concept is to account for phenomena that result from the interaction of smaller scale entities, such as physical factors, chemicals, species populations, and functional groups of populations. Examples are concentrations of chemical nutrients, population densities of component living species, various rate related measures such as productivities, and less easily quantitated concepts such as community structure. When these phenomena are viewed in the context of the whole ecosystem, i. e., not in an experimentally controlled situation, they are often referred to as whole system phenomena. Predicted ecosystem effects, as I shall refer to them, are standardized differences in whole system phenomena between a system in its undisturbed state and its state in the presence of a quantity of a particular toxic chemical. Effect can be quantified only against normal functioning; thus predicted ecosystem effect can be made only by contrasting the predicted affected state to the predicted normal state.

In predicting an effect, the same conditions are assumed for the normal as for the affected state, except that for the affected state the added presence of a toxicant is assumed. Predicted ecosystem effect is, therefore, conditional. Utility will depend both on the theoretical basis of the model and on the relevance of the conditions selected for the conditional mode analysis. The theoretical basis in the underlying disciplines of physics, chemistry, and biology, and the less structured discipline of hierarchial organization of the system representation is quite obviously a scientific question. Discussion of the theoretical basis occupies the bulk of this report. That the manner in which questions are asked of the model is also a problem for science is

less obvious. The problem of identifying, at least to my own satisfaction, the kinds of questions that one can logically expect to answer was a necessity for carrying out this research. I shall discuss this question also later in this report.

AQUATIC ECOSYSTEM

To predict effects of toxic chemicals in aquatic ecosystems several items are required. The most fundamental item is a clear definition of what effects are to be predicted. The term "aquatic ecosystem" must be defined specifically for the present purposes. As used in the assessment of ecological effects, the term can have one of two possible meanings. It can mean a particularly defined aquatic ecosystem (a single instance), or it can mean a range of defined aquatic ecosystems so that the effects of the toxicant over the range of systems can be referred more generically to "the aquatic ecosystem." In either case the term is used in conjunction with predicted ecosystem effects and, when so used, refers to the set of attributes that represent the aquatic ecosystem in the theoretical model. That is, one needs to realize that use of "the aquatic ecosystem" in conjunction with this model refers not to a physically identifiable environment, but to a set of attributes that relate abstractly to a set of attributes of real systems. The more substantial problem, however, is the provision of theory of ecosystem structure and function at a level of resolution to permit observation of the effects. Integration of information on toxicity of chemicals to aquatic organisms to the same level of resolution is a necessity. Finally, not only must both ecosystem theory and toxicity theory be organized at the level of resolution to permit observation of the effects, but each must be organized to interface with the other in a model to make the predictions of effects.

THEORY OF ECOSYSTEM STRUCTURE AND FUNCTION

Structure and function are inseparable in ecology. Structures enable functions. It is my assumption that there is parsimony of structure and behavior in biotic systems (an assumption in keeping with the principle of Ockam's razor): structures do not exist without function. Generally, this is a reasonable assumption, because power is required to maintain structures, and the competitive advantage is held by organisms without the added burden of useless structures. In the theory of ecosystem function proposed here the power demand is calculated as the net cost of carrying out the functions. It is assumed that there are no overhead costs for maintaining structure, except structure that is used in obtaining energy, survival, or reproduction. These assumptions are in keeping with the overall assumption of parsimony.

Much theory exists in ecology, in the generic sense of theory. This theory is diffuse, and it has not been assimilated at the

level of resolution that is useful for a theoretical model for predicting ecosystem effects of toxic chemicals, at least not in the vein of the model discussed here. The major effort in this research, therefore, has been to assimilate a theoretical basis for the model. In doing so I have held to the parsimony hypothesis. The level of resolution is such as to permit information on mode of action to be used when it is available, as well as to permit more general statistical measures of toxicity to be used. The ecosystem theory that is the basis of this theoretical model uses concepts from chemical thermodynamics (in much the same way as they are used in biochemistry), biochemistry, physiology, population dynamics, and limnology. A biophysical approach is used to derive relationships so that the resulting model equations are written primarily at the population level, with terms of the equations calculated using expressions reflecting underlying physiology, biochemistry, etc., all constrained by mass and energy accounting. Because reference is made to these finer levels in the describing equations, system effects at these levels also can be explored.

INTEGRATION OF ECOSYSTEM THEORY AND TOXICITY THEORY

Theory developed or assimilated in this research is primarily ecosystem theory. As noted, however, the ecosystem theory has been expressed so as to permit the application of various toxicity measures. Translation of LC_{50} values to effects on death rates in this model has the usual accompanying difficulties of interpreting LD_{50} values as rates and the additional difficulty of extrapolation to very low concentrations. Whatever the assumed interpretation and extrapolation mechanisms, the method of application of toxicity measures will be influenced by the approach taken in the model to represent ecosystem processes. This approach is to represent processes or functions as being carried out by a group of populations differing from each other in various ways, one of which is their susceptibility to a toxic chemical. The model does not represent particular existing species, but instead the model parameters are in the range of analogous values expected for existing species that carry out the process that is represented.

A fundamental assumption that amounts to a principle for this modeling approach is the basis for this non-specificity of representation. Simply stated, I assume that element cycling and most other macroscopic properties of ecosystems derive from interactions of organisms as they obtain useful energy via modes of metabolism suited to the energy sources. These modes of metabolism, unlike species, are common to diverse environments (see ECOLOGY AS THE ENVIRONMENTAL PATTERN OF BIOCHEMICAL ENERGETICS). I view a particular biotic community simply as a complement of species populations that are able to exploit the energy sources, grow and reproduce in a particular environment. This is not, I think, an extreme view. However, in a similar sense, for the model to be operational, computer algorithms are required to select coexisting species as represented in the

model. These are selected in the context of a given environment representation. It will be impossible for this environment to represent precisely any real environment, and by virtue of selection of species representations as a function of the environment descriptors, the species representations will not represent specific real organisms. For that matter, no one real environment can be said to represent precisely any other one, yet many organisms are common to widely different environments. Over time intervals relevant to selection processes, environments are not isolated and selection occurs over all communicating environments.

Derivation of the species representations, while not representing particular species, to maintain a credible level of reality, will use available information on appropriate existing organisms. Discussion of these matters, however, is very premature, because the working program is far from complete. The main ideas to derive from the comments are that this model is not directed toward any specific system representation, that on the contrary, a fundamental assumption is that the macroscopic system properties such as element cycling do not depend on any such specificity, and that perturbations (as by a toxic chemical) on a biotic community in a particular environment will result in characteristic alterations to the unperturbed behavior (see also CONCLUDING COMMENTS).

From a preliminary analysis on several compounds, considering all species together, toxicity can be represented by an asymmetric frequency distribution in which no taxonomic relationships above the species level are apparent. That is, if the frequency of occurrence of LC_{50} values (Criteria Documents Data Base 2,3) are plotted, the distribution is unimodal and skewed such that there is a low frequency tail at relatively high LC_{50} values. If one then identifies the species occurrence in this distribution, no pattern associated with taxa higher than the species level is apparent. These analyses are highly tentative, however, and another analysis with a much larger data base is beginning. Assignment of toxicities to the model populations with probability reflecting the frequency distribution appears to be a reasonable approach. In any case there is no basis to expect a close match between measured toxicities and the explicit needs of any ecosystem model, and therefore, no specific parameterization of a model can be expected. Use of toxicity information, therefore, will require that some rationale be employed; that employed here is to assign toxicities to the model as nearly as possible to match the measured frequency distribution. Use of this rationale, in general, will be limited by data availability, particularly for assignment of behavioral effects such as variation in hunting or escaping efforts.

MOTIVATIONAL BASIS

The motivation for this research project was the perceived need to be able to assess probable ecosystem effects, particularly effects on the cycling of major elements, resulting from the introduction of a toxic chemical. Such a capability would be most useful if it were prognostic and able to be used in an exploratory mode in search of generalizations about expected effects. Planning research to develop such a capability is an exercise in matching the possible forms of theoretical prediction with potentially useful questions. As a result of indulging in such an exercise I drew the following conclusions about some reasonable forms of useful questions, and what basis exists to support research toward providing answers to such questions using predictive models.

> Questions relating to effects on identifiable existing species in specific environments cannot be answered by a synthetic, predictive ecosystem model.
>
> It is feasible to answer questions relating to probable effects on ecosystem functions, given the following conclusions that a basis exists for a model of ecosystem functioning and effects of toxic chemicals on the functioning.
>
> > Enough is known of physical, chemical, biochemical, microbial, macro-organism biology, etc., to support virtually any level of underlying process description.
> >
> > Enough is known of ecological relationships to provide a basis for structural relationships in addition to those implied by the underlying process descriptions.

It is hypothesized (rather than concluded) that there is no dependency of system function on presence of particular species (as already discussed) nor on species diversity. Capacity of a system to carry out a process smoothly while populations involved in the process are stressed by a toxicant, however, depends entirely upon species diversity. The additional hypothesis is made that capacity for compensation increases at a decreasing rate as diversity increases. There is, therefore, dependency on the presence of species to carry out each function, and there is dependency on a minimal degree of diversity within each function to permit compensation by non-susceptible populations for reduction in population levels of species susceptible to toxic chemicals. The importance of this latter hypothesis to modeling the functional behavior of ecosystems using a multispecies representation, is that it is possible to represent ecological processes using a limited number of species, if it is true.

THEORETICAL BASIS

Following these ideas, a theory of ecosystem function was assimilated and work toward a functioning model based on the theory is in progress. The theory is not new in its entirety, but it does contain original elements. Perhaps more significantly, it departs from both holistic and reductionistic views. It departs from the traditional holistic view by attempting to synthesize system properties using a biophysical integration of finer scale components to the level required to represent the system. It departs from the reductionist view by concentrating on the ecosystem as the object to be represented and by virtue of interest in processes whose behavior cannot be considered to be a function of any single system component.

This theory like every theory of macroscopic phenomena, is based upon phenomenological models of its fundamental components. In an attempt to give the theory a greater predictive capability, I have selected as fundamental components, models representing energy transduction at the biochemical level. In these models organisms are considered as reaction systems that catalyze energy-rich, kinetically hindered redox reactions and, in the process, use part of the reaction energy for biosynthesis and mechanical work. Ultimately, population rates of change result from the biochemical models based upon redox chemistry. Ecological interactions result from dependencies among organisms for elements from which to form biomass and for compounds to serve as oxidation and reduction reactants to provide energy. To maintain the identity of all organic compounds that could serve as chemical nutrients or as energy substrates in the working model would be an impossible computing problem.

To overcome this problem, organic chemicals are aggregated into classes that are ecologically relevant. The underlying theory is worked out elsewhere (4) and does not depend on this aggregation. Toxic chemicals interfere with the processes by which organisms obtain or use energy or elements. Thus this theory of ecosystem function is based upon fundamental conceptual components that are models of real components that respond to toxic chemicals. Integration of toxicology at lower resolution, such as altered probability of death as obtained from reported LC_{50} values, can also be used directly without reference to the fine scale phenomenological models.

ECOLOGY AS THE ENVIRONMENTAL PATTERN OF BIOCHEMICAL ENERGETICS

ECOLOGICAL MODES OF METABOLISM. Disequilibria that drive biotic processes are in two forms: light and chemical. Organisms that use light induced disequilibria are phototrophs, and those that utilize chemical are chemotrophs (5,6) Phototrophy and chemotrophy refer to the source of energy, *i. e.*, whether the free energy is derived from photochemical or biochemical reactions. In either case the electron donor (reducing agent) can be either inorganic or organic (lithotrophy or organotrophy

with the prefix photo- or chemo-) making a total of four major classes of energy metabolism.

Figure 1 is a schematic of the processing of energy. For biosynthesis the source of carbon can be either CO_2 or organic compound (autotrophy or heterotrophy). Combining the modes of energy metabolism with the modes of biosynthesis, eight categories are formed, all eight of which exist in nature along with variations on these major categories. For the initial theoretical development, it will suffice to consider only three of the major categories: photolithoautotrophy, chemolithoautotrophy, and chemoorganoheterotrophy. Because there will be no risk of confusion, I shall refer to these categories by the shortened terms, photoautotrophy, chemoautotrophy, and heterotrophy. I shall further subdivide the latter category into macroheterotrophy and microheterotrophy, and microheterotrophy further into categories reflecting the electron acceptor used. I shall refer to these latter categories occasionally by the coarser terms, oxymicroheterotrophy and anoxymicroheterotrophy.

Figure 2 is a schematic of biosynthesis at the ecological scale. Figure 3 indicates the spatial and energetic relationships of microheterotrophy as a function of presence of potential terminal electron acceptors. Although too complex to represent graphically, a composite of Figures 1, 2, and 3 provides a rather complete, but abstract, scheme for element cycling.

ECOLOGICAL ENERGETICS. Energetics is simply a term for thermodynamics as applied to the analysis of biological processes. Biological processes, like all processes, proceed only when conditions of disequilibrium exist. More specifically, biochemical mechanisms proceed by transfer of electrons and associated energy to form, primarily, ATP and NADPH (or NADH). ATP is the universal mediator of biochemical reactions; NADPH and NADH are the major biochemical reductants. Processes in which these compounds participate are subcellular, yet processes by which they are formed and in which they are used are of utmost relevance at the ecological level of organization and of great utility in theoretical ecology. This is so because the macroscopic patterns in which they occur are interpretable, not at the cellular, individual, or population level -- but only at the ecological level of organization. That is, the existence of a particular mode of metabolism, for example -- chemoautotrophy, is a phenomenon that can be explained only with reference to ecological processes.

These processes are interactions of biotic and abiotic components that create and maintain environments suitable for particular modes of energy metabolism. Organisms can sustain a mode of energy metabolism in an environment only if the reaction on which this metabolism depends is thermodynamically favored (exergonic) in that environment. Specifically, organisms cannot maintain physiological conditions that permit a net derivation of energy from biochemical processes unless the net of those processes is

exergonic in their environment. This fact can be used as a major organizing principle for theoretical ecology. It provides the basis for calculation of potential modes of energy metabolism for given environmental conditions without reference to organisms.

The Gibbs free energy function is the appropriate measure for such calculations because it is a measure of the useful work that can be extracted from the energy of a reaction, and it refers to conditions of constant temperature and pressure, but allows volume to vary (as, for example, occurs in a biotic process that results in the evolution of a gas). These are conditions most appropriate to biological systems. Such calculations are not of energy budgets as such. Calculations for energy budgets usually consider that energy is conserved (in keeping with the first law of thermodynamics) and accountable when all system gains and losses are considered. Conservation of energy,thus, refers to conservation of the sum of all forms of energy. Energy that can be used by biotic systems is the Gibbs free energy for the specific energy yielding reactions, such as the oxidation of organic compounds with sulfate as the terminal electron acceptor.

The useful energy that can be extracted from these processes is a function of the concentrations of the reactants and products. Hence, ecologically relevant calculations for the amount of useful energy that can be derived from chemical reactions are functions of the conditions of the environments in which the reactions occur, and, hence, very definitely not subject to conservation laws. In contrast, however, mass conservation is a principle that is useful for theoretical ecological computations. In fact in the ecosystem model mass conservation is the fundamental principle for accounting that permits the calculation of the Gibbs free energy. This comes about because mass conservation is used directly as the accounting principle for calculating chemical quantities including concentrations, and the Gibbs free energy function for chemical reactions is dependent on concentrations of reactants and products.

AN ECOSYSTEM MODEL FOR ELEMENT CYCLING

An ecosystem model for element cycling is necessary for predicting effects of toxic chemicals on cycling processes. Morowitz (7) has shown that flow of energy through a system from a source to a sink will necessarily result in cycling in steady state systems. Ecosystems approximate steady state systems that are far from equilibrium, a condition that is associated necessarily with structure (8). The model presented here represents ecosystems as open systems that are far from thermodynamic equilibrium. The degree of approximation to steady state, however, is not explicitly assumed, but rather, the ecosystem is represented as a dynamic system. This is done because interest is in alterations in the rate of cycling, not

just in whether elements cycle. The fundamental basis for this model can be stated rather simply, but the details of these fundaments will occupy the next several pages.

The organisms that carry out the ecological modes of metabolism comprise the structures that are necessary for element cycle transformations. For each mode of metabolism, stability is maintained in part by diversity among the populations in their response to external factors. As a consequence of diversity, compensatory changes occur, resisting fluctuations in the fluxes of materials and energy that result from element cycle transformations. There is a high degree of similarity at the biochemical level within each mode of metabolism. Diversity exists in morphological variation and is expressed in physiological and behavioral differences. The development that follows is based on the foregoing assumptions of biochemical similarity and morphological diversity within metabolic modes.

The derivations and equations that follow, while comprising the greatest part of this report, should not be considered to be the most important part. They constitute my rationale for the way to express, ultimately in a computer model, the hypotheses and working assumptions already discussed. In attempting to develop a predictive model for aquatic systems without relying on the specifics of any one system, it has become apparent that traditional views of ecology present a barrier to the development of ecological theory. These traditional views, utilizing natural history and taxanomic approaches, have overemphasized, I believe, differences among ecosystems to the exclusion of theoretical approaches that do not assume from the outset the primacy of importance of specific taxa. This is not to claim that the approach put forth here has, indeed, overcome these barriers to the extent that a general ecological theory will result. Indeed, the approach that I present is also highly complex, dependent upon as yet unsupported hypotheses, and upon computational capabilities that could be very difficult to achieve. What I do claim, however, is that the viewpoint taken, which is more akin to that of microbial ecologists, is a valid one, and I should hope that if it does not lead directly to the goal of a model capable of predicting ecological effects, perhaps indirectly it will contribute to another approach that will.

A MODEL FOR UPTAKE AND FEEDING RATE WITH POTENTIAL LIMITATION BY SIMPLE SATURATION MECHANISMS

Every organism must cope with two problems, obtaining energy and obtaining elements from which to form biomass. Photoautotrophs potentially are limited in their energy supply rate by light availability because of light attenuation by various agents in water. For all microorganisms, obtaining chemicals from the environment is a process of molecular uptake of chemicals dissolved in water. There is a concentration gradient from the bulk water concentration to the concentration localized at the cell boundary. The gradient is generated when the cell removes dissolved material from the water at a rate that is competitive

with diffusional replenishment of the material at the external cell boundary.

These localized concentrations can limit the energy supply rate as well as the rate of supply of elements for biosynthesis. Macroheterotrophs either move through the water or move water past themselves to obtain food. Mobile organisms use energy for evasion of predators. In these activities the power to overcome drag can account for a considerable fraction of the total power expenditure. For large aquatic animals food supply for energy and biosynthesis must be maintained in an environment that is fluctuating with respect to food supply and pressure from predators. In the following the supply rate of energy and materials will be considered for each of the metabolic modes, and a resultant expression for population rate of change will be obtained.

It is usually assumed that the uptake rate of dissolved chemicals by microorganisms is best described by a rectangular hyperbola as first proposed for microbial processes by Monod (9). Such a description can be rationalized by any one of several specific mechanisms. All such processes appear to have a common characteristic, however, viz., a saturable component. In this respect many such processes exist, not all associated with microorganisms, and not all of which are biotic processes. Molecular sorption to particles is frequently described by the Langmuir isotherm, which, although not a rate description, is a rectangular hyperbola. In this instance the saturable component is the surface of the particle, or at least the capacity of the surface for the sorbate. The feeding of fishes was described in much the same way by Rashevsky (10) and the feeding of insect predators by Holling (11), the saturable component being the gut capacity in Rashevsky's analysis and available time in Holling's. Specifics of such processes will be discussed in the appropriate sections. The model is so generally applicable that it will be useful to indicate its derivation prior to specific uses.

The model consists of a description of each of two simultaneous processes: obtaining material (filling the saturable component) and removing material (restoring or emptying the saturable component). The rate of obtaining is proportional to the degree of unsaturation (S-x) and to the concentration of the material being obtained (s):

$$\frac{dy}{dt} = k_y s(S-x) \qquad (1)$$

The rate of change of material associated with the saturable component is the difference between the rate of obtaining and the

rate of emptying, the latter being proportional to the quantity of material associated with the saturable component:

$$\frac{dx}{dt} = \frac{dy}{dt} - k_e x \tag{2}$$

In the above, y is the material being obtained, x is the same material in the saturable component, S is the capacity of the saturable component, and k_o and k_e are rate constants for obtaining and emptying, respectively.

For large populations over time intervals long with respect to characteristic times for the two processes, the degree of saturation will reach a stable value, implying that the rate of emptying is equal to the rate of obtaining. Thus

$$\frac{dy}{dt} = k_e x \tag{3}$$

from which

$$x = \frac{Ss}{k_e/k_u + s} \tag{4}$$

Substituting into equation 3 gives the expression for the rate of obtaining material when the processes are at a steady state:

$$\frac{dy}{dt} = \frac{k_e S s}{k_e/k_u + s} \tag{5}$$

TRANSPORT LIMITED CHEMICAL UPTAKE RATE

Even though microorganisms move, it is not clear what stimuli result in the movement, what terminates movement, whether movement ceases upon reception of other stimuli, etc.. There is difficulty, therefore, in representing activity of microorganisms as a function of their energetic needs. It is more convenient to consider activity as part of the fundamental metabolism of microorganisms. As noted one aspect of microorganism physiology that is a result of size and the related absence of morphological features for feeding is the uptake of dissolved chemicals from the environment. For very small organisms viscosity of water is high enough that movement results in little advantage in terms of increased food availability. Diffusion and other mixing processes, threrefore, are important in bringing food to the organism (12, 13).

The rectangular hyperbola is assumed to be the appropriate description of uptake of dissolved chemicals from the

environment. Depending upon characteristics of the environment and the organisms, depletion of the chemical in the immediate vicinity of the cell surface can reduce the uptake rate below that expected when depletion is not considered. Pasciak and Gavis (14, 15) and Gavis and Ferguson (16) analyzed this problem. Their model for the influence of local depletion of dissolved chemicals on uptake rate accounts for the effects of cell size and shape. If s is replaced by C_b, the concentration of the chemical at the cell boundary, and S by M, the capacity of the cell membrane for the chemical in moles cm^{-2}, then equation 6 represents a flux onto the cell membrane (Figure 4). This flux can also be described in terms of Fick's first law:

$$J_b = -3.6D(C - C_b)R^{-1} \tag{6}$$

where J_b is the flux at the cell membrane, D is the diffusivity of the chemical in water ($cm^2\ sec^{-1}$), C is the bulk concentration, R is the cell radius, and conversion to moles cm^{-2} hr^{-1} requires the conversion factor, 3.6. The flux to a spherical cell is equation 6 multiplied by 4 R^2:

$$4\pi R^2 J_b = -14.4\pi RD(C - C_b) \tag{7}$$

When the two expressions for the flux into the cell (equations 5 and 7) are equated, a quadratic in C_b is obtained. Pasciak and Gavis (14) write this equation in non dimensional form as

$$C_b^2 + (P^{-1} + 1 + C)C_b - C = 0 \tag{8}$$

where $C_b = k_u C_b / k_1$, $C = k_u C / k_1$, and $P = 14.4\ RD/k_u$. C_b is available via the quadratic formula and resubstitution of the above.

To account for cell geometries other than spheres, Pasciak and Gavis (15) modified the above results to represent oblate and prolate spheroids (disks and spindles). This is accomplished by multiplying P by a shape factor that is a function of the eccentricity of the cells (eccentricity is a measure of the relationship of the major and minor axes). For a complete description and derivation see Pasciak and Gavis (15) and their references.

This description of the uptake process is rather general, permitting uptake to be represented for any micrroorganism that uses dissolved substances. It does not provide, however, a description of uptake by aufwuchs or benthic communities. This is easily accomplished by a development similar to the one described above, but using a rectangular coordinate system. In this solution the concentration at the surface of the community depends upon the thickness of the unstirred layer adjacent to the

surface. Accuracy of uptake calculations depends strongly upon knowledge of the thickness of this layer.

AUTOTROPHY

Photosynthetic production of biomass and O_2 coupled with aerobic respiration form a complete element cycle. Respiration in light and diffusion limited environments depletes O_2, and consequently other oxidizing agents are used. These conditions are usual in deep waters, organically rich waters, wetlands and soils. Each oxidizing agent, like O_2, participates in a cycle that is complete. These redox cycles, mediated biologically for the elements of interest here (C, O, N, P, and S), form the basic structures of the biogeochemical or element cycles. Chemoautotrophs obtain energy from oxidation of reduced inorganic compounds, usually with O_2 as the oxidizing agent (terminal electron acceptor, TEA). Elements that are reduced during anaerobic respiration are oxidized during chemoautotrophy, thereby completing the cycle. These processes occur in different environments, however, and therefore transport is a key process in the cycles and potentially is the limiting step.

Most chemoautotrophs are gram negative bacteria of pseudomonad related genera (17) and are, therefore, prokaryotes. Photoautotrophy is carried out predominantly by green algae and cyanobacteria. Green algae are eukaryotes and cyanobacteria, prokaryotes. It might be expected that extreme diversity of biochemical function exists among such diverse kinds of organisms. In regard to energy metabolism and biosynthesis (Figure 5), however, there is little diversity. The Calvin cycle is the mechanism for fixation of CO_2 and production of hexoses (17) Lehninger (18) gives the following reaction for biosynthesis in photoautotrophs:

$$CO_2 + 2H_2O + 2H^+ + 3ATP + 2NADPH \rightarrow (CH_2O) + 3P + 3ADP + 2NADP^+ \quad (9)$$

Here (CH_2O) refers to 1/6 of a hexose. The degree to which the reaction is favored thermodynamically can be seen by decomposing it into its three component reactions.

$$\begin{aligned} ATP + H_2O &\rightarrow ADP + P & \Delta G^\circ(w) &= -7.3 \\ NADPH + \tfrac{1}{2}O_2 &\rightarrow NADP^+ + H_2O & \Delta G^\circ(w) &= -52.5 \\ CO_2 + H_2O &\rightarrow (CH_2O) + O_2 & \Delta G^\circ(w) &= 114.8 \end{aligned} \quad (10)$$

When the standard free energies are used the net free energy for the reaction is -12.12. Under physiological conditions, however, the reaction is probably even more favorable. An indication of this can be obtained by introducing only the free energy of ATP hydrolysis (-12.5 kcal M^{-1}) reported by Burton (19). This increases the tendency of the reaction to proceed ($\Delta G(w) = -27.72$). The analogous reaction for chemoautotrophic bacteria differs only in the use of NAD^+ and NADH rather than $NADP^+$ and NADPH (17). The energetics are approximately the same.

Diversity of autotrophy lies neither in energy metabolism nor biosynthesis but in the sources of energy: light for the photoautotrophs and a very large variety of redox reactions for the chemoautotrophs. Table 1 gives several of the reactions used by chemoautotrophs as energy sources.

MODELING AUTOTROPHIC ENERGY METABOLISM AND BIOSYNTHESIS. The strategy that I have adopted for representing autotroph growth is similar for both photoautotrophs and chemoautotrophs. Energy, whether light or chemical, and chemicals for biosynthesis have to be obtained separately. Therefore, energy or any element can limit the growth rate at a given time. My strategy is to calculate the growth rate that could be sustained on the supply rate of each required factor (element or energy), if no other factor were limiting. That is, given the concentration or density of a resource, the rate at which it can be obtained and used assuming that nothing else limits the use rate is calculated. This produces a set of potential resource limited growth rates. The actual growth rate is then taken to be the minimum of this set.

LIGHT LIMITED GROWTH OF PHOTOAUTOTROPHS IN AQUATIC SYSTEMS. Suspended substances reduce light by shading and dissolved substances by frequency selective sorption. The Beer-Lambert law expresses the reduction in intensity with depth (or mean optical path) as a function of a situation specific attenuation coefficient, ϵ:

$$\frac{dI}{dz} = -\epsilon I \tag{11}$$

Units of the rate are E absorbed m^{-2} of surface area m^{-1} depth day^{-1}, the units of I are E m^{-2} day^{-1}, and of the characteristic attenuation coefficient, ϵ, are m^{-1}. Steele (20) proposed an equation for the rate of photosynthesis as a function of light intensity:

$$p = p_m \left(\frac{I}{I_m}\right) e^{1 - I/I_m} \tag{12}$$

where p_m is the maximal rate of photosynthesis, reached when the light intensity is I_m. Equations 11 and 12 can be combined for the rate expected at any depth, etc., when the parameters are known.

Bannister (21) developed production equations in terms of a parameter that is more closely related to the biochemical processes of energy gathering and utilization, ϕ_m, the maximal quantum yield. Bannister's analysis was carried out in terms of productivity, $\underline{M}(C)\ m^{-3}day^{-1}$. It perhaps would be a purer analysis to express the quantum yield in terms of electron moles E^{-1}, and to work in terms of electron equivalents throughout the model. At this point, however, it would introduce an extra and apparently unnecessary step, and so I shall use Bannister's analysis including his units. He used three separate light curve equations. Because it includes the photoinhibition effect, I shall use Steele's equation (20, 21) as equation 12 above. The derivation is given here in abbreviated form.

Reduction of light with depth can be partitioned into reduction by each of the causal components. Reduction rate by suspended algae is caused primarily by the absorption of light by the cellular pigments. The molar adsorption rate is

$$\frac{dI(A)}{dz} = k_a A I \tag{13}$$

with units of E absorbed $m^{-3}day^{-1}$ (actually to be in keeping with the units of the derivative with respect to depth the units might better be expressed as E m^{-2} of surface $day^{-1}m^{-1}$ of depth). Normally productivity is measured in g(C) $m^{-3}day^{-1}$ or equivalent. Division by 12 converts to moles. The quantum yield is expressible as the ratio of the molar productivity to the molar adsorption rate, with units of $\underline{M}(C)\ E^{-1}$, and an explicit expression for the quantum yield can be obtained by substituting from equations 12 and 13.

$$\frac{P}{12} \Big/ \frac{dI(A)}{dz}\ ;\ \phi = \frac{P_m e^{1 - I/I_m}}{12 I_m k_a A} \tag{14}$$

As light intensity approaches zero, saturation effects on the photopigments disappear and the quantum yield approaches a maximum:

$$\phi_m = \frac{P_m e}{12 I_m k_a A} \tag{15}$$

This quantity theoretically is a constant, its value in natural waters being approximately 0.06 (21) or 0.07 (22) in units of $\underline{M}(C)\ E^{-1}$ absorbed. Substituting for I in equation 12 and integrating with respect to depth gives the total photosynthesis rate per unit surface area. Further substitution for p_m (from

equation 15) and for ϵ in terms of the light attenuation factors provides the total photosynthesis rate in terms of parameters and the chlorophyll concentration, A. If this rate is integrated over time, production is obtained. To do so requires that I_0 be written as a time dependent light flux. This can be approximated in several ways, but is not represented here.

The quantity that is needed for the simulation approach taken here is the depth-integrated photosynthesis rate of carbon assimilation, considering no limiting factors besides light. Two depths are of interest: either a given depth as, for example, is of interest when a volume element of particular dimensions is considered, or the compensation depth given by the depth at which the light compensation point is reached. In either instance the applicable equation for photosynthesis rate is

$$P_T = 12 \phi_m I_m e^{-I/I_m} (L-1) A / (\frac{k_w}{k_a} + A) \qquad (16)$$

in which L is the fraction of the incident light that is transmitted through the element, and is given by

$$L = I'/I_m = e^{-(k_w + k_a A) z'} \qquad (17)$$

If z' is a fixed depth, equation 17 can be used, but if z' represents the compensation depth, then the light level, I', at the compensation depth must be specified, and L is calculated directly as $L = I'/I_m$.

Equation 13 is the primary equation for calculating light-limited rate of growth of photoautotrophs. In simulation calculations it may prove convenient to express the rate as a quantity per volume, rather than per surface area. This is a simple multiplication of the quantity , p_T, by the applicable surface area to which the total applies.

ENERGY LIMITED GROWTH OF CHEMOAUTOTROPHS IN AQUATIC SYSTEMS. Energy is obtained for chemoautotrophy by uptake of reduced inorganic chemical species and of oxygen as an oxidizing agent, and by carrying out the redox reaction. Both the chemicals that are used for the energy reaction and those that are used in biosynthesis are obtained by uptake through a gradient. Therefore the concentration at the cell membrane can be the limiting factor (equation 8). The chemical that is used as the electron donor in the energy reaction can also be used as a

substrate for biosynthesis. For example in nitrifying bacteria the following reaction is used for energy:

$$NH_4^+ + 3/2\ O_2 \rightarrow NO_2^- + H_2O + 2H^+ \qquad \Delta G^\circ = -69.94 \quad (18)$$

Ammonia is also used for synthesis. It must be supplied at a rate that is commensurate with the other needs of growth, and therefore, the rates at which it is required for energy and for synthesis each need to be calculated and compared to the other needs. Equations 9 and 10 apply equally well to all autotrophs. From these equations it can be seen that three moles of ATP and two of NADPH are required to synthesize one mole of carbon. Using standard free energy values, this requires that at least 126.9 kcal be supplied via the above reaction (equation 18). Assuming 38% efficiency (the same as is often calculated for photoautotrophs (23) and heterotrophs (18), 334 kcal from about 5 moles of NH_4^+ must be released (a quantum yield of 0.2 $\underline{M}$ carbon synthesized $\underline{M}^{-1}$ NH_4^+ utilized for energy). A quantum yield of 0.2 was observed by Gunderson and Mountain (24). It can be seen that for energy to be a non limiting commodity, ammonia must be obtained at five times the rate of obtaining CO_2 and at 3 1/3 the rate of obtaining O_2. The same kinds of calculations apply to each of the energy reactions indicated in Table 1.

THE ACHIEVED GROWTH RATE OF AUTOTROPHS. The above kinds of comparisons are valid if autotroph growth is resource limited, a situation that is expected in all but unusual transient conditions. Energy and all chemicals can be present transiently in abundant supply. Under these conditions growth is limited by some inherent intracellular property. Growth rate is then maximal, and the condition is transitory because the populations that are growing maximally increase rapidly until some resource again becomes limiting. I shall assume that the minimum of the maximum uptake rates, as limited by membrane transport, is the growth limiting factor for autotrophs. That is, the maximal growth rate that is achieved under these conditions is the minimum of the growth rate that would be achieved maximally for each of the required resources. By this assumption it is not necessary to provide a separate growth model for this special case, because it is calculated naturally as the limit of the general case.

The general case of growth is the minimum of the growth rates that would be achieved on each of the required resources. Elemental composition of the organisms has to be considered when calculating these minima, however. One way to accomplish this is to reference each of the rates to the carbon assimilation rate. If the organism's elemental composition is $C_cN_nP_pS_s$, then the ratio of nitrogen to carbon is n/c, nitrogen is required at only n/c dC/dt, and thus the minimum of dC/dt and c/n dN/dt would be the expected growth rate if either carbon or nitrogen were limiting (here and in the following equation dC/dt and dN/dt are

used to indicate the uptake rates of C and N). In general the growth rate is given by

$$\min\left(E, \frac{dC}{dt}, \frac{c}{n}\frac{dN}{dt}, \frac{c}{p}\frac{dp}{dt}, \frac{c}{s}\frac{dS}{dt}\right) \quad (19)$$

Each of the rates of assimilation is described by an equation like equation 5.

HETEROTROPHY

Heterotrophs derive both energy and biomass from a complex mixture of chemicals. Some fraction of this mixture is essentially indigestible. The remainder is hydrolyzed to small compounds and further broken down to small monomers (7) Some of the monomers are used as reactants for energy production and some for biosynthesis. Essentially any of the monomers can be used for energy, but in biosynthesis discrimination among monomers must occur so that biomass specific to the particular heterotroph can be synthesized. This general scheme characterizes the metabolism of both microheterotrophs and macroheterotrophs. Microheterotrophs, of course, deal with the complex organic mixture extracellularly first, then after it is broken down into soluble compounds, absorb it and use it for energy and synthesis. Excretion of products that cannot be used for energy or synthesis is an important process for microheterotrophs. Macroheterotrophs consume complex organic mixtures either as other organisms or as detritus, and the whole process of digestion and metabolism is carried out internally. Elimination of indigestible material and breakdown products that cannot be used for energy or synthesis are both important processes for macroheterotrophs.

A MODEL FOR CALCULATING GROWTH RATE OF HETEROTROPHS. The above description of the growth and energy metabolism of heterotrophs is a simplification, whose purpose is to establish the categories of organic chemicals that I shall employ to represent growth of heterotrophs. In keeping with the overall objective of representing ecological processes that are important in element cycling, the growth model will be a function of the supply rate of each of the important elements. As already discussed these processes are driven by redox disequilibria, created by photoautotrophy and providing continual input to the respiratory (redox) processes carried out by heterotrophs in obtaining energy. The model for calculating growth rate consists of three parts. One is the component for partitioning of food into power supply and biomass synthesis. A second is the calculation of power demand. The other is the calculation of food consumption rate in terms that permit calculation of power supply as well as the supply rate of food components whose composition is similar to that of the consumer.

PARTITIONING OF FOOD INTO POWER SUPPLY AND BIOSYNTHESIS. Food consumption, power consumption, power production, and biosynthesis are rates. The problem faced by heterotrophs is to obtain food at a rate so that the power produced from it satisfies the power demand of obtaining food and escaping predators plus the basic power demand of life processes and repair with enough remaining power and materials to support growth. Figure 6 gives the scheme for accounting the energy and materials in partitioning the food intake rate into power output and biosynthesis. The scheme refers most directly to macroheterotrophs, but it is applicable to microheterotrophs if food is considered to consist of dissolved organic chemicals and elimination of the indigestible fraction is ignored. Figure 7 shows the assumed relationships of the categories of organic chemicals in the aquatic system. Processes and states inside the dashed line occur inside microbial cells.

The object of the model is to calculate growth rate of a heterotroph population. This is accomplished in several steps. Composition of the food is compared to the composition of the heterotroph so that the rate of consumption of two food components can be calculated. The two components are biomass-like (referenced as pool 1 in the following) and non biomass-like (pool 2). (The term "pool" should be interpreted to indicate a dynamic quantity characterized by varying elemental composition as the composition of food varies.) In the overall model, the free energy content of total food at any time is known via an accounting chain. The free energy content of each pool is calculated as part of the function of this model as is discussed below. This provides the power supply via each of the two pools. The disposition of the pools is determined by comparison to the power demand, and growth rate is immediately available as a result of this comparison. The specifics of the process are given below in the sequence of the descriptive overview presented in this paragraph.

The process of partitioning food into power supply and biosynthesis is developed in the following in terms of macroheterotrophs. The situation for microheterotrophs is simpler in one aspect because of the representation as lumped categories of the organic chemicals on which they feed. The development for macroheterotrophs can be applied to microheterotrophs by considering the categories of organic in place of the species of prey. But in another aspect it is more complex. Macroheterotrophs use a single electron acceptor, oxygen, whereas microheterotrophs use a whole series of them. Use of the term "energy content" is to be interpreted as the free energy of the reaction between a chemical serving as an electron donor and another chemical serving as an electron acceptor. In much of the following the electron acceptor is assumed to be oxygen and no single chemical will serve as electron donor, but rather electrons will derive from a mixture of chemicals, comprised of the biomass of higher organisms. In this situation

also, I shall use the term "energy content." A discussion of energetics with electron acceptors other than oxygen will follow the section on food partitioning.

The food intake rate (Mass t^{-1} consumer^{-1}) is

$$F_{\cdot j} = \sum_i F_{ij} \tag{20}$$

where i indicates a source of food (prey population or environmental pool of chemical), and j identifies the predator. The overall elemental composition of an organism (or of a chemical pool can be represented for the elements of concern as

$$C_c O_o N_n P_p S_s \tag{21}$$

where the upper case letters symbolize the elements as usual, and the lower case letters represent the mole numbers of the elements with which they are associated. Let n_{ik} represent the mole number of element k, species i, and w_k represent the gram atomic weight of element k. Then the fraction of food mass obtained from prey species i comprised of element m is

$$f_{im} = \frac{n_{im} w_m}{\sum_k n_{ik} w_k} \tag{22}$$

so that the rate of consumption of element m in the mixed food is

$$F_{\cdot jm} = \sum_i f_{im} F_{ij} \tag{23}$$

The average molar rate of consumption of elements by consumer j is the set

$$\left\{ \frac{F_{\cdot jc}}{12}, \frac{F_{\cdot jo}}{16}, \frac{F_{\cdot jn}}{14}, \frac{F_{\cdot jp}}{31}, \frac{F_{\cdot js}}{32} \right\} \tag{24}$$

Division of each of the elements of this set by the mole number of the consumer for the corresponding element gives another set, the least value of which corresponds to the element of the food which is in least supply relative to the composition of the consumer. A set of mole numbers for the composition of the food normalized to the element in least supply can be obtained by dividing the elements of the set of molar consumption rates (equation 24) by the rate for the element in least supply. A similar set can be obtained for the consumer by dividing the mole numbers of the consumer empirical formula by the mole number of

the element in least supply. Then the food can be partitioned into the two pools. The normalized empirical formula of food can be represented as

$$C_{c_F} O_{o_F} N_{n_F} P_{p_F} S_{s_F} \tag{25}$$

and, because pool 1 is like consumer biomass, it can be represented as

$$C_{c_j} O_{o_j} N_{n_j} P_{p_j} S_{s_j} \tag{26}$$

In the above formulae, the subindex F indicates that the mole numbers are for the food, and the subindex j indicates that those mole numbers are for pool 1 which is like consumer j. Pool 2 component constitutes the remainder of food. Its mole numbers are the difference between the mole numbers of the food and of pool 1:

$$C_{c_F - c_j} O_{o_F - o_j} N_{n_F - n_j} P_{p_F - p_j} S_{s_F - s_j} \tag{27}$$

Now the rate of consumption of the two pools can be calculated. First let n_{kj} represent the mole number of element j in pool k. Conservation requires that

$$\sum_j n_{Fj} = \sum_j (n_{1j} + n_{2j}) \tag{28}$$

The fraction of food that is pool k is

$$f'_k = \sum_j n_{kj} \Big/ \sum_u n_{Fu} \tag{29}$$

and the rate of consumption of pool k (k = 1 or 2) is

$$F'_{.jk} = f'_k F_{.j} \tag{30}$$

If the free energy content of food is known, then it too can be partitioned. Morowitz (7) discussed some of the problems of using free energies of biological materials and concluded that enthalpy (heat content) values are useful approximations. There are other approaches to this problem that could yield better approximations, but that problem will be left, and I shall merely assume at this time that free energy values are available.

The free energy content of food can be obtained if the free energy content of individual food items is known:

$$\Delta G_{Fj} = \frac{\sum_i \Delta G_{ci} F'_{ij}}{\sum_k F'_{kj}} \qquad (31)$$

G_{ci} is the free energy content of species i.

During the process of digestion of the food to monomers, a small loss of free energy occurs, the polymer bond energy, ΔG_d. The free energy of pool 1 is the same as the free energy of the consumer less the free energy loss of depolymerization, $\Delta G_{m1} = \Delta G_{cj} - \Delta G_d$. Pool 2 free energy is the remainder less the energy loss of depolymerization: $\Delta G_{m2} = (\Sigma F_{ij} \Delta G_F - F_1 \Delta G_{cj})/F_2 - \Delta G_d$. The power supply from the two pools can now be calculated. From pool 1 it is

$$P_{m1} = F_1 \Delta G_{m1} B_j^{-1} \qquad (32)$$

where B_j indicates the mass of an individual of species j, and from pool 2 it is

$$P_{m2} = F_2 \Delta G_{m2} B_j^{-1} \qquad (33)$$

Describing the way that this free energy is used to produce ATP and NADPH requires a model of cellular biochemistry. I assume that discrimination between the two pools occurs, so that pool 2 is used preferentially for energy and pool 1 as material for biosynthesis. Power demand, P_a is taken to be the sum of the energy expense rates for maintenance, repair, motility of hunting and escaping, and other activities associated with feeding. If the power demand is greater than power production from pool 2, then pool 1 is used as needed. If the power demand is less than power production from pool 2, then pool 2 remainder is converted into new biomass at at rate determined by the uptake of the necessary inorganics to achieve the consumer's elemental composition or it is converted into storage compounds. The remainder, in excess of the rate of conversion by these processes, is eliminated. Four distinct cases arise as a result of the comparison of the power supply and demand:

Case 1: pool 2 power supply > power demand for activity plus synthesis of pool 1 into consumer biomass:

$$\phi_c P_{m2} > (P_a + F_{ij} \Delta G_p B_j^{-1}) \phi_s^{-1} \qquad (34)$$

Case 2: pool 2 power supply > power demand for activity but < power demand for activity plus synthesis of pool 1 into consumer biomass:

$$P_a \phi_s^{-1} < \phi_c P_{m2} < \left(P_a + F_{1j} \Delta G_p B_j^{-1}\right) \phi_s^{-1} \quad (35)$$

Case 3: pool 2 power supply < power demand for activity, but pool 1 + pool 2 power supply > power demand for activity:

$$\phi_c P_{m2} < P_a \phi_s^{-1} < \phi_c \left(P_{m1} + P_{m2}\right) \quad (36)$$

Case 4: pool 1 + pool 2 power supply < power demand for activity:

$$\phi_c \left(P_{m1} + P_{m2}\right) < P_a \phi_s^{-1} \quad (37)$$

In the above ϕ_c represents the efficiency of obtaining free energy during the catabolic process, ϕ_s the efficiency of use of the free energy in activity or biosynthesis, and ΔG_p the free energy required for polymerization of the monomers into biomass.

Specific (per capita) growth rates can be calculated for each of the above cases.

Case 1: all of pool 1 is synthesized, and the growth rate, therefore, is

$$\mu_j = \frac{dB_j}{B_j dt} = F_{1j} B_j^{-1} \quad (38)$$

$$P_{m2r} = P_{m2} - \left(P_a + F_{1j} \Delta G_p B_j^{-1}\right) \phi_c^{-1} \phi_s^{-1}$$
$$F_{2r} = P_{m2r} B_j \Delta G_{m2}^{-1} \quad (39)$$

Remaining pool 2 can be synthesized at a rate determined by uptake of necessary elements, or it can be turned into storage compounds. These processes are not discussed further here.

Case 2: pool 2 supplies the power demand of activity plus part of the power demand of synthesis. The growth rate on pool 1 monomers sustained by power derived from pool 2 is

$$\mu_{j2} = \phi_c \phi_s \left(P_{m2} - P_a\right) \Delta G_p^{-1} \qquad (40)$$

Power to synthesize the remainder of pool 1 must derive from pool 1, itself. The remainder of power in pool 1 is

$$P_{m1r} = P_{m1} - \mu_{j2} \Delta G_{m1} \qquad (41)$$

Thus, the growth rate sustained by the remainder of pool 1 is

$$\mu_{j2} = \phi_c \phi_s \left(P_{m2} - P_a\right) \Delta G_p^{-1} \qquad (42)$$

The net growth rate is the sum of the two, which after simplification is

$$\mu_j = P_{m1}\left(\Delta G_p + \phi_c \phi_s \Delta G_{m1}\right)^{-1} + \phi_c \phi_s \left(P_{m2} - P_a\right) \Delta G_p^{-1} \qquad (43)$$

Case 3: pool 2 is insufficient to supply the power demand of activity, so pool 1 is diverted at the necessary rate. The power available from pool 1 remainder is

$$P_{m1r} = \phi_c \left(P_{m1} + P_{m2}\right) - P_a \phi_s^{-1} \qquad (44)$$

The growth rate that is sustained on pool 1 remainder is

$$\mu_j = \phi_c^2 \phi_s \left(P_{m1} + P_{m2} - P_a\right)\left(\Delta G_p + \phi_c \phi_s \Delta G_{m1}\right)^{-1} \qquad (45)$$

Case 4: the power obtainable from the total food is less than the activity power demand. It is assumed that the consumer continues to attempt to carry out normal activities of feeding, escaping, etc., at the expense of body mass. The

net effect to the whole population is a loss of biomass, expressible as a negative growth rate:

$$\mu_j = \phi_c (P_{m1} + P_{m2}) - P_a \phi_s^{-1} \qquad (46)$$

The growth rates calculated above (equations 38, 43, 45, and 46) use values for power production rate and power utilization rate, in addition to the patterns of physiological processes and biomass composition. Power is used at the cellular level, but it can be accounted most easily at higher levels of organization. Power is required for biosynthesis, hence the accounting point is in the model for biosynthesis, i. e., in the above equations describing growth. There are two other major categories of power demand. One is the basic metabolic demand. The other is the demand due to motile activity. This latter demand is more readily accounted at a higher hierarchial level, the power required to move a body through a liquid medium. Power production rate is a function of the composition of the food, and of the rate at which it is obtained. Hence, a description of the feeding process is an important part of the model, because in its development the basis will be obtained for calculating power supply, supply of materials for biosynthesis, motile activity for obtaining food, and motile activity for escaping predators. In addition loss rates caused by predation are obtained by simple rearrangement of the equations for feeding.

FEEDING BY MACROHETEROTROPHS. Macroheterotrophs capture discrete food particles by one of two general means. Either they feed upon all particles encountered that are within the size range that they can handle, or they select and capture individual food particles by explicit overt action. I shall refer to organisms characterized by the former behavior as filter feeders and to those by the latter as pursuit feeders.

The derivation for uptake and feeding given in equations 1 - 5 follow the general pattern of Rashevsky's (10) derivation of stationary state feeding rate for fishes. His work was motivated by Ivlev's (25) studies on the feeding of fishes. Ivlev's model for fish feeding is widely used in mathematical models of systems that include feeding by large consumers. It was derived as a formal mathematical expression that fitted his data. Rashevsky derived his model from assumptions about the way that fishes feed. Part of his purpose was to present a stationary state analysis based on Ivlev's model, which described the feeding of of fishes as a function of the density of food. Ivlev's equation was of the form

$$R = R_m (1 - e^{-z B_w}) \qquad (47)$$

where R is the food eaten per experiment (a fixed time), R_m is the maximum feeding rate for the fixed time, B_w is the biomass

density of prey (mass per volume), and z is a fitted constant.

Rashevsky's derivation of an equation comparable to Ivlev's began with the statement that the feeding rate (F) equals the encounter rate (E) times the probability that the prey is eaten if encountered (P):

$$F = E\ P \tag{48}$$

The encounter rate is derived by assuming that the predator sweeps out a right circular cylindrical volume as it swims in search of food. The encounter rate is then the product of this volume per time and the density of prey in the volume, r^2vB, where r is the radius of the cylinder, v is the swimming velocity, and B is the mass of the prey per volume of water. Rashevsky took the probability of consumption given an encounter to be proportional to the unfilled gut capacity, an assumption exactly equivalent to that made in equation 1.

The latter assumption is credible for situations in which the saturable component is filled via mechanisms that operate passively, such as the adsorption of dissolved chemicals onto a microbial cell membrane. Where the component is filled by active processes, however, such as the filling of a fish's stomach by active feeding, it is not clear that the rate of filling is necessarily proportional to the unfilled capacity. If the probability that an individual consumes a prey increases as unfilled stomach capacity increases, but not linearly, then this model better approximates the feeding of a population where there is a distribution of the extent of filling than it does an individual's feeding. Ivlev's fits of the model to data indicated no discrepancy from the model of direct proportionality, however, and therefore, the point is more cautionary than substantial. The point should simply be borne in mind that it is not necessary for a higher organism to reduce its feeding rate to the fraction of its maximum that corresponds exactly to the fraction of unfilled stomach capacity. In this particular regard the model of Rashevsky and the models that are developed here are not necessarily based upon an unassailable assumption.

The encounter rate is

$$E = \pi r^2 v B_w \tag{49}$$

where r is the encounter radius, v is the swimming velocity, and M_w is the biomass density as in Ivlev's model. The probability of consumption of prey given an encounter is

$$P = c(M_s - M_g) \tag{50}$$

where M_s is the capacity of the stomach, M_g is the quantity of food in the stomach, and c is a constant of proportionality. If the probability of consumption is 1 when the gut is empty ($M_g = 0$) then the proportionality constant, c, is M_s^{-1}. Thus the feeding rate is

$$F = \pi r^2 v B_w \left(\frac{M_s - M_g}{M_s}\right) \tag{51}$$

Feeding rate, F, is the same as the rate of change of stomach content, dM_g/dt if the experiment is done over a short enough time interval that stomach emptying can be ignored (there is no loss term). Integrating and putting $M_g = 0$ when $t = 0$, the stomach content is

$$M_g = M_s \left(1 - e^{-\frac{\pi r^2 v B_w t}{M_s}}\right) \tag{52}$$

For Ivlev's experiment, $t = t_f$, the fixed experimental length, so that the constant, z, of Ivlev's model is equivalent to $\pi r^2 v t_f / M_s$ of Rashevsky's. As noted by Rashevsky (10), Ivlev's model applies only to the phenomenon of feeding as a function of concentration of food. That is, it does not take into account other factors that affect feeding, such as stomach emptying rate. It is not suitable, therefore, for use in a model in which time intervals are long enough that the other factors become important.

For a population considered over a time interval that is long compared to the characteristic times for stomach filling and emptying, the mean food intake rate equals the mean stomach emptying rate, *i. e.*, steady state feeding is achieved:

$$\pi r^2 v B_w \left(\frac{M_s - M_g}{M_s}\right) = k M_g \tag{53}$$

where k is the stomach emptying rate constant. The feeding rate is obtained by rearranging Equation 53 so that kM_g is expressed

in terms that do not include the stomach content, M_g, and recalling that at steady state feeding, feeding rate equals the stomach emptying rate, or

$$F = \frac{k M_s B_w}{\frac{k M_s}{\pi r^2 v} + B_w} \tag{54}$$

Note that this equation is of the same form as Equation 5, and that its equivalent components are interpretable similarly.

To the extent that this model represents the main features of predator-prey interactions in aquatic systems it has a property that is very useful, it permits complete specification of predator-prey interactions as a function of the characteristics of the individual predator and of the population densities of predator and prey. That is, no species specific, pairwise interaction coefficients are needed. Immediately, however, one rejects that predator-prey interactions involve characteristics of the predator and not the prey. In the following a more detailed derivation of predator-prey models is made for two major ecological modes of feeding by aquatic organisms, filter feeding and pursuit feeding. In these models characteristics of both predator and prey are incorporated while retaining the characteristic that no interaction coefficients are required.

FILTER FEEDING. Consumers that feed indiscriminantly upon all organisms that they encounter that are within the size range possible for them to feed upon are grouped here under filter feeders. It is assumed that they move through the water creating a disturbance front detectable by prey with suitable sensory organs. Some of these prey are able to escape and some are captured. The scheme for this type of feeding is given in Figure 8. If a prey organism swimming at velocity v_p swims normal to the path of the oncoming predator, reaching the edge of the encounter cross section, the distance $\rho - r$, before the predator swimming at velocity v_c swims the encounter distance s_d, then the prey escapes; else it is captured. All distances, τ, such that

$$(\rho - \tau)/v_p = s_d/v_c \tag{55}$$

are escape distances. All prey inside the radius, τ, at the point of encounter with the disturbance front preceding the predator are captured. The feeding rate of an individual predator feeding on a single prey of population density, M, is

$$F = \frac{k M_s \tau^2/\rho^2 B}{\frac{k M_s}{\pi \rho^2 v_c} + \frac{\tau^2}{\rho^2} B} = \frac{k M_s B}{\frac{k M_s}{\pi \tau^2 v_c} + B} \tag{56}$$

The first of the two forms of F, although somewhat more cumbersome, is preferable, because it groups quantities together

that are properties of the predator alone. Hence, in dealing with several prey populations and one predator these quantities are constants. They are the factor, kM_s, and the whole first term in the denominator. The second of the two forms indicates that the effective rate that the predator hunts is dependent upon both predator and prey. That is in the first the volumetric search rate is $\pi\rho^2 v_c$, but in the second the comparable term is $\pi r^2 v_c$, a smaller quantity that is a function of both predator and prey because r is a function of the swimming velocities of both. The expression for feeding by predator j on n prey populations is

$$F_j = \frac{\frac{k_j M_{sj}}{\rho_j^2} \sum_i^n r_{ij}^2 B_i}{\frac{k_j M_{sj}}{\pi \rho_j^2 v_{cj}} + \frac{1}{\rho_j^2} \sum_k r_{kj}^2 B_k} \qquad (57)$$

PURSUIT FEEDING. Consumers that swim at one velocity while searching for prey, then pursue the prey at another velocity are referenced here as pursuit predators. Figure 9 gives the schematic for this mode of food gathering. The searching velocity of the predator is v_{cj}. The distance at which the predator can detect prey is taken here to be a constant that is characteristic of the predator, s_{dj}. It can be made a function of water clarity or even a function of prey size or other characteristic without major change in the form of the derivation. Upon detection both predator and prey begin swimming at the pursuit velocity, v_{pj}, and flight velocity, v_{fi}, respectively. The duration of the pursuit, t_{pij}, is given by

$$t_{pij} = s_{dj} / (v_{pj} - v_{fi}) = s_{dj} / \Delta v_{ij} \qquad (58)$$

The prey's distance of the flight, s_{fij}, is given by

$$s_{fij} = v_{fi}\, s_{dj} / \Delta v_{ij} \qquad (59)$$

It is arbitrarily assumed that prey that escape swim the same distance as prey that are captured, and similarly for predators. Another arbitrary (but necessary for simulation) function was developed (but not discussed in detail here) to calculate the probability of escaping pursuit predators. Essentially it is assumed that the probability of escape is greater, the closer is v_{fi} to v_{cj}. That is if the prey can swim nearly as fast as can the predator, there is a high probability of escape.

As with filter feeders the effective rate that the pursuit predator hunts is a function of both predator and prey. Gerritsen and Strickler (26) developed a model for predation that depends on both predator and prey cruising velocities. This

model is equivalent to the effective hunting rate, the rate of encounters while hunting:

$$a_{ij} = \pi s_{dj}^2 \left(\frac{u^2 + 3w^2}{3w} \right) \tag{60}$$

where $u = \min(v_{ci}, v_{cj})$, $w = \max(v_{ci}, v_{cj})$, and v_{ci} and v_{cj} are the cruising velocities of prey i and predator j, respectively. The rate of encounters while hunting is greater than the feeding rate, because pursuit feeders spend their time in two ways, searching and pursuing. (In general I shall aggregate all activities involved in feeding into pursuing, i. e., pursuit, capture, handling, ingestion. First, however, it is less cumbersome to develop the model in terms of overall rate of encounter, then later to introduce the probabilities of pursuit given encounter and of capture given pursuit.)

In parallel to the phenomenon of partitioning a saturable component into filled and unfilled portions, a pursuit predator partitions time into searching and capturing:

$$F^*_j = (T_s + T_p)^{-1} \tag{61}$$

where F^*_j is the encounter rate, T_s is the mean time spent searching per encounter, and T_p is the mean time spent pursuing per encounter. More specifically the mean search time per encounter and the mean pursuit time per encounter are

$$T_s = \left(\sum_i a_{ij} N_i \right)^{-1} ; \; T_p = \sum_i R_{ij} t_{pij} \tag{62}$$

where R_{ij} is the relative frequency of the ij^{th} encounter:

$$R_{ij} = \frac{a_{ij} N_i}{\sum_k a_{kj} N_k} \tag{63}$$

After rearrangement the encounter rate can be written as

$$F^* = \frac{s_d^{-1} \sum_g \Delta v_{gj} \sum_i a_{ij} N_i}{s_d^{-1} \sum_k \Delta v_{kj} + \sum_l a_{lj} N_l} \tag{64}$$

Unlike the expression (Equation 57) for filter feeders, the components of Equation 64 are not as simple dimensionally as is desirable for ease of interpretation. The terms of the denominator each represent an encounter rate, the first relating to pursuits and the second to detections of prey while the

predator is searching. If the equation is rewritten by dividing both numerator and denominator by the sum of the velocity differences, the "half saturation" term becomes simply the detection distance for an encounter, a form that is perhaps more easily interpreted. Without exhausting the possible ways that the equation could be rewritten in search of a form that is most readily interpretable, it is apparent that the components of the expression are functions of characteristics of both predator and prey to a greater extent than are the comparable components of Equation 57. It is therefore comparably more difficult to separate the components of the equation in such a manner that it is as easily interpreted.

To complete the model for pursuit predation, the effect of stomach filling must be incorporated. In the general expression for the limitation of feeding rate by stomach filling (Equation 51), the probability of feeding was taken to be proportional to remaining stomach capacity. A similar assumption is made here. The encounter rate times the probability of encounter for pursuit feeders is the encounter rate, F^*, as developed above times the probability of feeding given an encounter, $(M_{sj} - M_{gj})/M_{sj}$. At steady state feeding this rate equals the stomach emptying rate, kM_{gj}:

$$F_j = kM_j = F^*\left(\frac{M_{sj} - M_{gj}}{M_{sj}}\right) \tag{65}$$

Rewriting to remove terms involving the variable, M_{gj}:

$$F_j = \frac{kM_{sj}F_j^*}{kM_{sj} + F_j^*} \tag{66}$$

Equations 57 and 66 are expressions for feeding rate of the two major ecological modes of feeding by macroheterotrophs. By parameter variation they can be made to describe a wide variety of behavior by these types of organisms. For example, Equation 66 can be made to describe the feeding of an ambush predator by noting that the cruising velocity of such a predator is zero, which reduces the expression for the volumetric search rate to $a_{ij} = \pi s_{dj}^2 v_{ci}$. An additional consideration is the feeding of macroheterotrophs in communities in which there is a wide disparity in sizes of the organisms present. Introduction of a factor in the numerator of both equations to account for the size window within which feeding occurs overcomes the potential problem for an operating model. The function that I have used expresses the probability of ingestion as a function of prey size. I shall not describe it in detail in this report.

Expressions can be obtained for mortality occurring in a population as a result of consumption by populations of filter and pursuit feeding predators, and for power used in moving about in the activities of feeding and escaping being fed upon.

MORTALITY CAUSED BY PREDATION. The mortality rate experienced by a population is the sum of the mortalities caused by all the predators. The quantity, therefore, is obtained by summing the rates over all predators. One approach is to consider that the mortality caused by a predator population, j, on a prey population, i, is the total feeding rate of the predator multiplied by the fraction that the specific prey population comprises of the total prey encountered by the predator. The appropriate fraction, however, is not simply the prey population mass divided by total prey mass of all species. The appropriate expression is obtained by using the encounter radii, τ_{ij}, as weights, so that the fraction corresponds to the proportion of total encounters that occur with the prey population i. For filter feeders it is

$$f_{ij} = \frac{\tau_{ij} B_i}{\sum_k \tau_{kj} B_k} \tag{67}$$

The mortality to i caused by j is

$$m_{ij} = f_{ij} F_i \tag{68}$$

and the mortality to i caused by all predators combined is

$$m_{if} = \sum_j f_{ij} F_j = B_i \sum_j \frac{\frac{k_j M_{sj} \tau_{ij} B_j}{k_j M_{sj}}}{\pi v_{cj}} + \sum_k \tau_{kj} B_k \tag{69}$$

where m_{if} is the mortality rate to population i caused by filter feeding predators. This expression can also be arrived at by perhaps a more direct approach. Consider the expression for F_j, equation 57. This equation is a sum of n terms, any specific term of which refers to the portion of food that derives from a particular prey population. If an expression is formed that consists of the sum of specific terms for population i, one from each feeding rate expression (57), then equation 69 results directly.

For pursuit feeders essentially the same approach is used, except that encounter rate constants (equation 60) are used as weighting factors. The resulting expression is

$$\frac{\dfrac{k_j M_{sj}}{s_{dj}} \sum_u \Delta V_{kj}}{s_{dj}^{-1} \sum_\ell \Delta V_{\ell j} + k M_{sj}} a_{ij} \Bigg/ \frac{\dfrac{k M_{sj}}{s_{dj}} \sum_r \Delta V_{rj}}{s_{dj}^{-1} \sum_h \Delta V_{hj} + k_j M_{sj}} + \sum_u a_{uj} B_u \qquad (70)$$

where m_{ip} is the mortality rate to population i caused by pursuit feeders.

POWER DEMAND RESULTING FROM MOTILE ACTIVITY. The power required to move around in a viscous fluid nominally is porportional to the third power of the velocity of movement:

$$P = \frac{1}{2} C_D \delta A V^3 \qquad (71)$$

where C_d is the drag coefficient, δ is the density of water, A is the appropriate area of the moving organism, and V is velocity. The drag coefficient, C_d, is not a constant, however, but is a complex function of velocity. In practice C_d has to be measured as a function of the velocity (or the Reynolds number) for each shape (13). This difficulty of operation will not be discussed further here. Instead, it is assumed that equation 71 is sufficient to develop the ideas for the model, thereby deferring this operational difficulty until the time when parameter values are sought for the model.

A heterotroph does not swim at constant speed, so its power demand is a variable. I assume that a heterotroph's time can be partitioned into four kinds of activities: searching, pursuing, escaping, and inactivity. (Filter feeders do not pursue, so for them this fraction is zero.) If every individual in the population behaves in this way, and the behavior is not synchronous, nor correlated time-wise, then an alternate view is that the fractions refer to the fractions of the population engaged in the four activities at any time. I have not taken into account a time fraction spent in reproductive activities as would be appropriate for higher organisms. There is, however, allowance for energy of reproduction in the cost of biosynthesis (see PARTITIONING OF FOOD INTO POWER SUPPLY AND BIOSYNTHESIS). A rationale for accounting power expenditure for reproductive activities could possibly begin by partitioning the power that now is allotted to growth into a portion for activities associated with reproduction (nesting, migrations, etc.) and a portion for population growth. Unfortunately, no means is apparent to me at this time by which to rationalize this partitioning, and a great deal of research would necessarily precede such a model. It

would be necessary to determine whether any relationships exist, for example, between power availability and the elaborateness of reproductive behavior. As represented in the present model, any unaccounted activity will result in calculation of growth rates greater than could be attained in reality.

To obtain the fractions, I have assumed that an organism's first priority is self preservation. Therefore the fraction of time spent escaping predators can be calculated independently of all the other fractions, and the other fractions simply partition the remaining time. A given organism can be subject to predation by both filter feeders and pursuit feeders. The fraction of time spent escaping predators, in general, will be a function of both types of predation. The fraction of time remaining for feeding after escaping predators, in general, will alter feeding behavior, and equations 57 and 66 must be correspondingly corrected to account for this effect.

Calculations of these fractions of time make use of the relationships already developed. When all ramifications are considered, however, they are more tedious than is worthwhile for presentation in this report. Therefore they will not be presented in detail. Instead the general approach taken in obtaining the derivations will suffice.

The fraction of time spent in an activity is the time per unit (or event) of that activity times the rate of occurrence of that activity. Thus the fraction of time spent escaping predators is the time per escape times the encounter rate. (Naturally, the actual calculation is far more involved. For example, one complication is that the fraction of time spent fleeing is calculated as the difference between the fraction of time spent being pursued and the fraction of time spent being captured, because the power used by those that are captured is irrelevant to the surviving population.) After the fraction of time spent escaping, f_e, is accounted, the remaining time, f_r, is partitioned into feeding and inactivity. The expressions for feeding are corrected for reduction in available time by escaping predators by noting that stomach emptying occurs at the same rate regardless of the predation pressure, while feeding itself is limited to the remaining time. The power required for the activity is obtained by multiplying the velocity of swimming in each activity by the fraction of time spent in each activity and using equation 71 for organism j in the following form

$$P_j = \tfrac{1}{2} C_{D_j} \cdot \delta A_j \sum_k \left(f_{kj} v_{kj} \right)^3 \qquad (72)$$

where f_{kj} is the fraction of time spent in the kth activity by organism j, and v_{kj} is its velocity in that activity.

At this point power supply via feeding, power demand as a function of activity, and disposition of the elements comprising the food are all calculable for heterotrophs using the

relationships developed. One additional aspect of metabolism needs to be considered for theoretical completeness, so that a closed system of equations can be developed to represent element cycling. That aspect is the use of different oxidizing agents as terminal electron acceptors in the energy metabolism carried out by all heterotrophs.

ENERGY METABOLISM AS A FUNCTION OF TERMINAL ELECTRON ACCEPTOR. To represent organic chemicals in a general way as sources of materials for energy and synthesis, it is necessary to group them into categories. Criteria for establishing these categories include similarity of elemental composition, energy content, and the way in which organisms use them. These criteria do not specify the level of resolution, however, and in the final analysis the categories will be selected through experience with attempts to match several possible categorization schemes with the other model components to achieve the results with reasonable economy. An initial scheme is presented in Figure 7. In this scheme the categories are particulate organic matter (POM), refractory organic matter (ROM), digestible organic matter (DOM), soluble organic matter (SOM), itself consisting of two components: biomass-like monomers (BOM) and non-biomass-like monomers (NOM). POM receives input from organism deaths, molts, egesta, etc. The distinction between ROM and DOM is purely categorical, i. e., no process separates ROM from DOM. DOM, however, is readily hydrolyzed by exoenzymes of microorganisms into SOM, whereas ROM is only very slowly solubilized. SOM is absorbed by the organisms, and separation into BOM and NOM occurs. (This is also a categorical distinction as discussed in the section on partitioning of food into power supply and biosynthesis.) This categorization scheme reflects the mode of biological utilization more explicitly than similarity of composition or energy content. It is possible that for the latter criteria additional categories will be required. It might become necessary, for example, to represent CH_4, acetate, or other specific categories of chemicals that are important in microbial systems for the model to reflect certain aspects of their dynamics.

As organisms oxidize organic chemicals for energy, there is a sequence of utilization of electron acceptors that corresponds to the variation in redox potential for the reactions (4, 27). That is, a preferred electron acceptor is used until it is depleted, then the next preferred form is used, and so on. O_2 is used first, followed by NO_3^{-1} and NO_2^{-1}, SO_4^{-2}, and CO_2. Other oxidants are also used, such as other forms of sulfur. The interesting point of this sequence is that the preferred sequence is in the order of the energy released in the reactions. Oxidations of organic compounds using the more preferred electron acceptors result in greater energy yield than reactions using the less preferred. It is unlikely that this reflects any chemical necessity (4), but more likely reflects the competitive advantage accruing to organisms that use the more highly productive energy sources. This sequence of reactions will be expressed wherever

transport or regeneration of electron acceptors is slower than their use by organic decomposition. In natural systems, it is expressed temporally in highly eutrophic systems and spatially as vertical stratification in systems with highly organic sediments, such as wetlands and many water bodies.

The use of oxidants in sequence can be represented by the assumption that the strongest oxidant present is used. The problem that then remains is that of calculating the energy yield appropriate to the oxidant that is being used. One direct approach to this problem is that suggested as appropriate by McCarty (4), the use of half reactions and equivalent weights as described in elementary chemistry texts, and as is commonly used in biochemical calculations (28, ch. 17). If this approach is taken the standard free energies of the half reaction of their reduction (at pH 7, and unit activity for the other reactants), per equivalent weight of the oxidants is in the order corresponding to the sequence of their utilization. An exception to this is nitrite, whose value for $\Delta G^{o}(w)$ is higher than that of O_2. It is not clear whether this apparent reversal in tendency is a consequence of adaptation of the organisms that use nitrite as an electron acceptor or of the peculiar relationship of nitrite to nitrate. That is, nitrite is formed as a product of nitrate reduction and is available as a reactant, therefore, only after nitrate is reduced.

For the scheme for representing organic matter to be used effectively, an accounting algorithm must be applied to enforce the conservation of mass. The algorithm that is applied here is in outline the following. Each of the categories of OM are treated as state variables, except that POM is not represented as a separate state variable, but rather as a sum of DOM and ROM. Fractions of the various sources of detritus are refractory to hydrolysis and are therefore ROM. The remainder is DOM. DOM is lost through hydrolysis to soluble compounds, SOM, which in turn is lost via uptake by microorganisms. As discussed above, the subsequent processes are as represented for macroheterotroph metabolism. Conservation of mass in this model, however, has a more specific meaning. The elements of concern must be individually conserved. This is accomplished by accounting the concentration of the elements in each of the pools. The rules given above then apply to the individual elements. The pools are treated in many respects as a single type of molecule with mole numbers proportional to the concentrations of the elements. (Except that for computations using the Gibbs free energy, it is not assumed that the concentration of the molecule as a reactant is that of the whole pool. See Energetics above.)

The above procedures will guarantee conservation of mass, but to calculate the energy yield from reaction with the various oxidizing agents requires an additional algorithm. The oxidants are represented as half reactions in which an electron equivalent of the oxidant plus an electron (hence electron acceptor) yields a reduced form of the element. A complementary half reaction is required for the electron donor, a molecule from one of the

categories of organic matter. This can easily be done (but is not discussed here). Of more difficulty is the problem of obtaining the appropriate free energy for this half reaction. The approach to be taken initially is to use a conservation rule for heat of combustion with oxygen so that the energy of the pools is accounted dynamically. When calculating the energy yield for reaction with another oxidizing agent, the reaction with oxygen will be replaced by an equation for the appropriate reaction by first removing the half reaction for oxygen and then substituting the half reaction for the oxidizing agent of interest.

MODEL SUMMARY

The above several sections summarize a complete and theoretically rationalized basis for a multi-species, yet functionally oriented, ecosystem model. It yet remains for this theory to be implemented into a working computer model. Further work is needed to provide a basis for describing physiological, behavioral, population level, and other specific effects with a comparable degree of theoretical rationale. It is quite possible that this work will require yet additional work on the model as presented.

CONCLUDING COMMENTS

MACROSCOPIC METAVIEW AND MICROSCOPIC APOLOGIA

The futility of the reductionist method for studying systems has often been argued convincingly. Early in this report I noted that I have departed from both the holistic and reductionistic approach. Yet it has not surprised me to find that many with whom I have discussed these ideas have gained the impression that this research is extremely reductionistic. They have noted that it is reductionistic to attempt to understand a natural system by studying its parts in detail, and that this approach to ecology, historically has failed. They have further noted that my work bears a strong resemblance to that approach. There is a great philosophical and operational difference, however, between this model and the reductionistic approach.

This model is indeed constructed of fine scale components. But in contrast to the failures to comprehend natural systems through comprehensive study of their parts, I expect to obtain predictions at the ecological scale. The reason for optimism can be explained by contrasting the comprehensibility of natural and engineered systems. Engineered systems are understood essentially as well as their component parts are understood, because they have been explicitly designed and constructed. Oftentimes models are constructed of mathematical analogs of the component parts and coupled in a way considered to be analogous to the way that the engineered system is built. The model is itself an engineered system, built in strict analogy to the physical engineered system. It is intended that the model output

represent the system level behavior of the engineered system. The degree to which the model behavior actually represents that of the physical system depends upon the closeness of the analogies between the systems, which in turn depends upon the skill of the modeler. There is no question of whether any failure of the model to describe the physical system's behavior is due to inherent impossibility of obtaining system level behavior from a model constructed of mathematical analogs to fine scale physical components.

All coupled models, including the one discussed in this report, are engineered systems. At issue is whether this model's behavior will represent, to any useful extent, behavior of natural systems. Specifically not at issue, as argued above, is whether system behavior can result from a model constructed of fine scale components. As with models of engineered system, the extent to which model behavior will represent natural system behavior will depend upon the closeness of the analogies between model components and physical couplings.

Physical ecosystems are comprised of a virtual infinitude of components. It is patently obvious that it is impossible to study or represent all of them. But even if it could be done, one would have a representation of only a single ecosystem. Patterns of ecosystem behavior for broad categories of systems are recognizably similar, even if not predictably so. There is structural and functional similarity that apparently emerges, in the presence of significant diversity of system components. Analogously, a system model, if constructed of components that well represent the processes that occur in a type of ecosystem, can be expected to exhibit functional behavior similar to that of the system type whose components are represented, despite the unavoidable misrepresentations of the greatest majority of species present in physical ecosystems.

The manner in which I anticipate that this model's system behavior will represent real system behavior is best explained in terms of three macroscopic, testable hypotheses about this model and its relationship to natural system behavior. It is my hypothesis that it will be possible to find complements of species representations (sets of attributes) that will coexist for very long times (not necessarily asymptotic coexistence), and further that among such coexisting complements that there will be a high degree of similarity of process rates. That is, I hypothesize that there may be many nearly stable model communities that could occupy a model environment, but that one will not be able to discriminate among them merely by considering differences in process rates. Further, I hypothesize that the predicted ensemble average ecological effect of a specific toxicant will not differ distinguishably among such coexisting complements. A connection with reality is needed for these results to be considered predictions, and the final hypothesis provides this connection. I hypothesize that one will not be able to discriminate between measurements on processes occurring in a real system and analogous values of processes as calculated

by this model, including the ecological effects of toxic chemicals, provided that the real system's boundary conditions can be well represented in the model. This latter provision recognizes that uncertainty in boundary conditions can limit the capability to discriminate between the predictions and observations. Laboratory ecosystems hold some promise of overcoming this potential limitation by permitting control over boundary conditions so that they can be represented in the model.

If these hypotheses are borne out, and calculational difficulties can be overcome, then this model will provide a synthetic means of predicting ecosystem effects. If they are refuted, the results will suggest other hypotheses.

SCALE OF RESOLUTION, REDUCTIONISM, HOLISM, AND PREDICTED ECOSYSTEM BEHAVIOR

The third hypothesis is the critical one. Underlying this hypothesis is the premise that interactions of the equations will be analogous to interactions among real ecosystem components. In fact the results of any ecosystem model must depend upon the same premise, regardless of whether they are considered reductionistic or holistic. The equations of any model must bear some relationship to the system components that they represent. The degree of resemblance is dependent on the correspondence of the level of resolution to the resolution of the components of the natural system components of interest, and on the skill with which these components have been selected and described. If a fine scale of resolution is selected, a model is apt to be called reductionistic, or conversely, if coarse, then holistic. But is the difference between reductionism and holism merely a quantitative difference in scale of resolution? I would argue that scale of resolution is not even relevant to the distinction between the two views. If one is interested in studying the response of processes or entities as a function of the level or intensity of various influences, where the uncontrolled fluctuations of the system have been "reduced" to an acceptable level, then the view is reductionistic. If, on the other hand, one is interested in processes or entities that take on their special characteristics as a result of the direct and indirect influences of other system components, then the view is holistic. Moreover, taking a holistic viewpoint does not necessarily admit a coarse scale of resolution. The scale of resolution dictated by the processes and entities of interest, whether the viewpoint is reductionistic or holistic.

There is no intent for this model to reproduce the detailed behavior of a real physical system in such a manner that one could identify the behaviors of real living species in the results. What is intended is that this model be an analog of aquatic systems, in the sense that system behaviors that cannot be attributed to individual biotic species, i. e., whole system properties, are indistinguishable from results of the same kinds of behaviors of natural systems with similar boundary

conditions. The possibility that such results can be obtained depends on the choice of processes to represent, the adequacy of the description of those processes over the operating range, and the application of constraints (conservation laws, thermodynamic and kinetic principles) in a manner that is analogous to constraints on natural systems.

All results of a system model must necessarily be viewed as system level results. There are two categories of system level results, however. One is the sort that could also be measured in a reductionistic way in a controlled experiment, for example -- a chemical reaction, but whose peculiar characteristic in the system context results from system interactions. The other is the sort that cannot be observed in a reductionistic way, because it does not exist apart from the system. An element cycle is an example of such a result, and measurement of the flow of material around an element cycle loop is an example of a system level measurement.

The distinction is not as great as it might at first appear, however, because of the possibility of interpreting the former sort of result as indicative of the latter. Patterns of interactions are new macroscale phenomena that arise via the existence of the system, but they can be observed only at the scale of observation possible for the observer. Thus measurements of chemical reaction rates in the system can be observed and used to infer behavior of the whole pattern of the element cycle in which it participates. It is not inconceivable that some sort of observation could be made at the scale of the pattern itself. It is characteristically human to perceive and discriminate among patterns, but it is quite another level of difficulty to quantify objectively patterns of behavior in a manner to permit discrimination among behaviors of ecosystems. If the capacity for this sort of perception and discrimination among ecosystem behaviors is to be developed, it would appear that models of about the complexity of that described here would be valuable in the endeavor.

Energy Processing Cycle

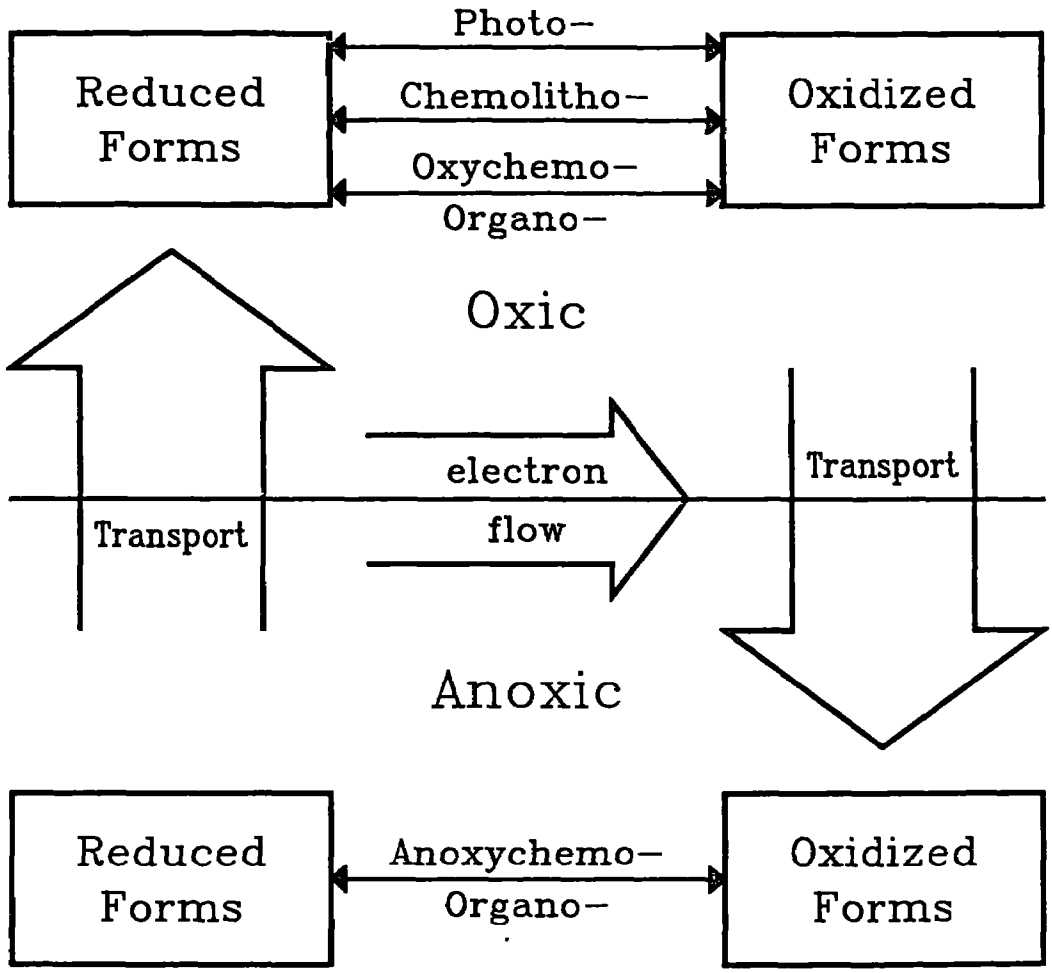

Figure 1. Schematic for redox processes that yield energy useful for biotic processes. Elements cycle between reduced and oxidized forms.

Biosynthesis

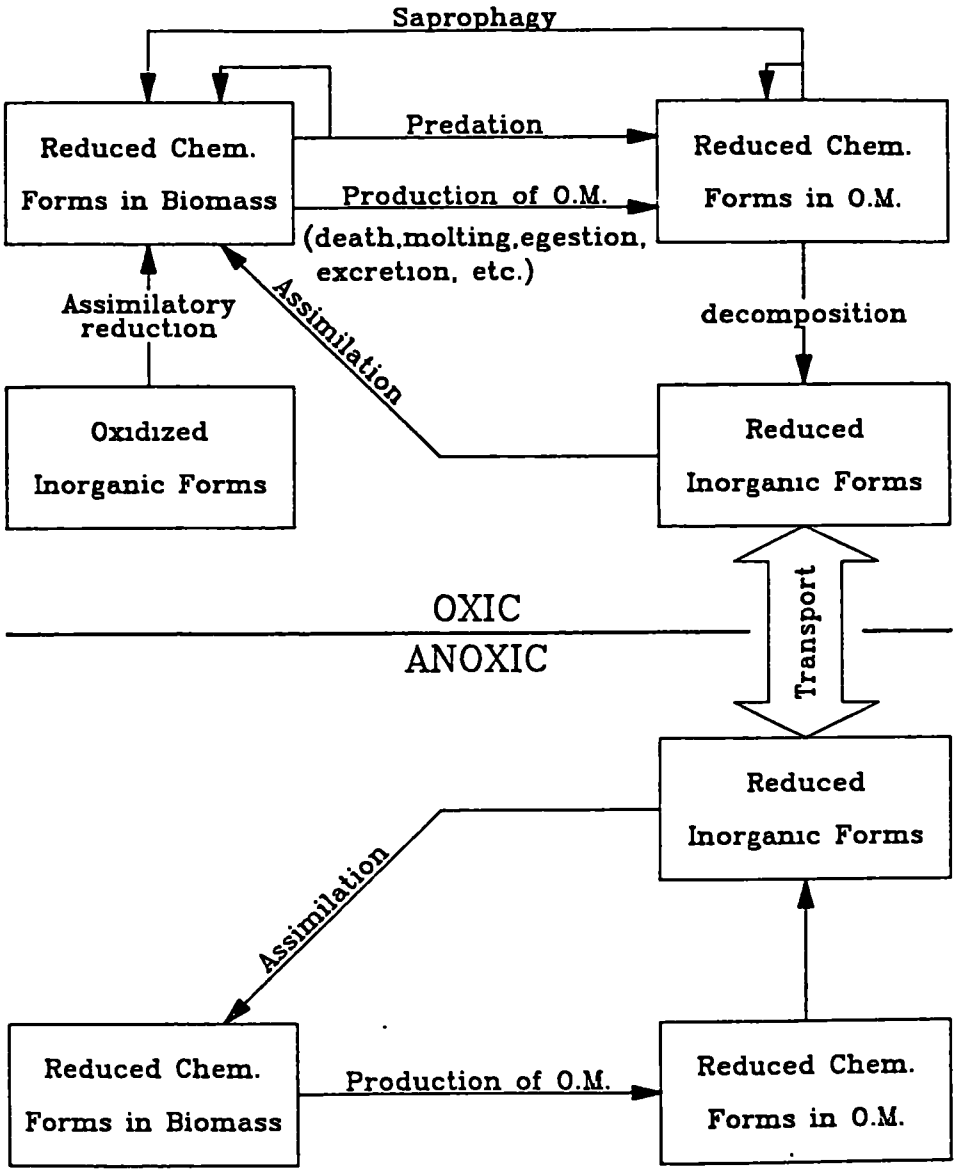

Figure 2. Relationships among chemical and biotic forms of elements in biosynthesis.

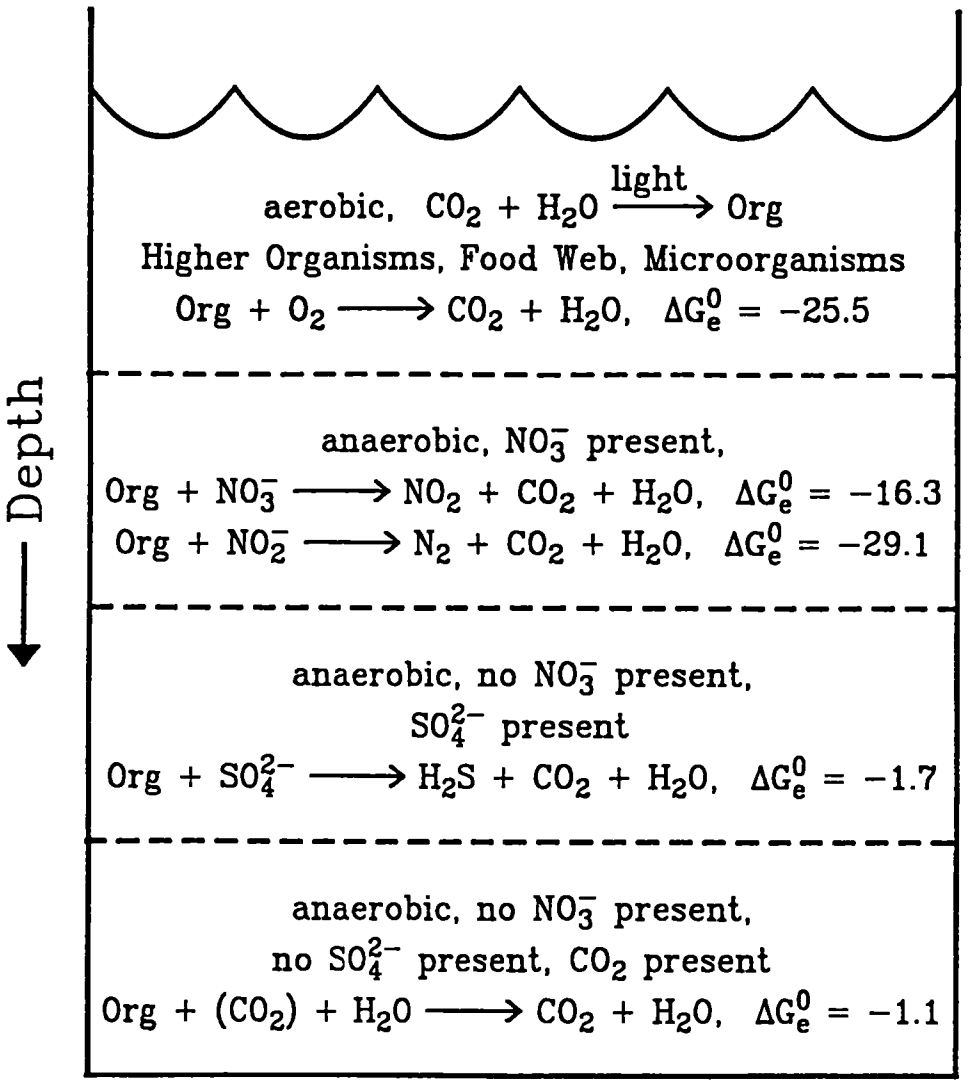

Figure 3. Variation in terminal electron acceptor as function of depth.

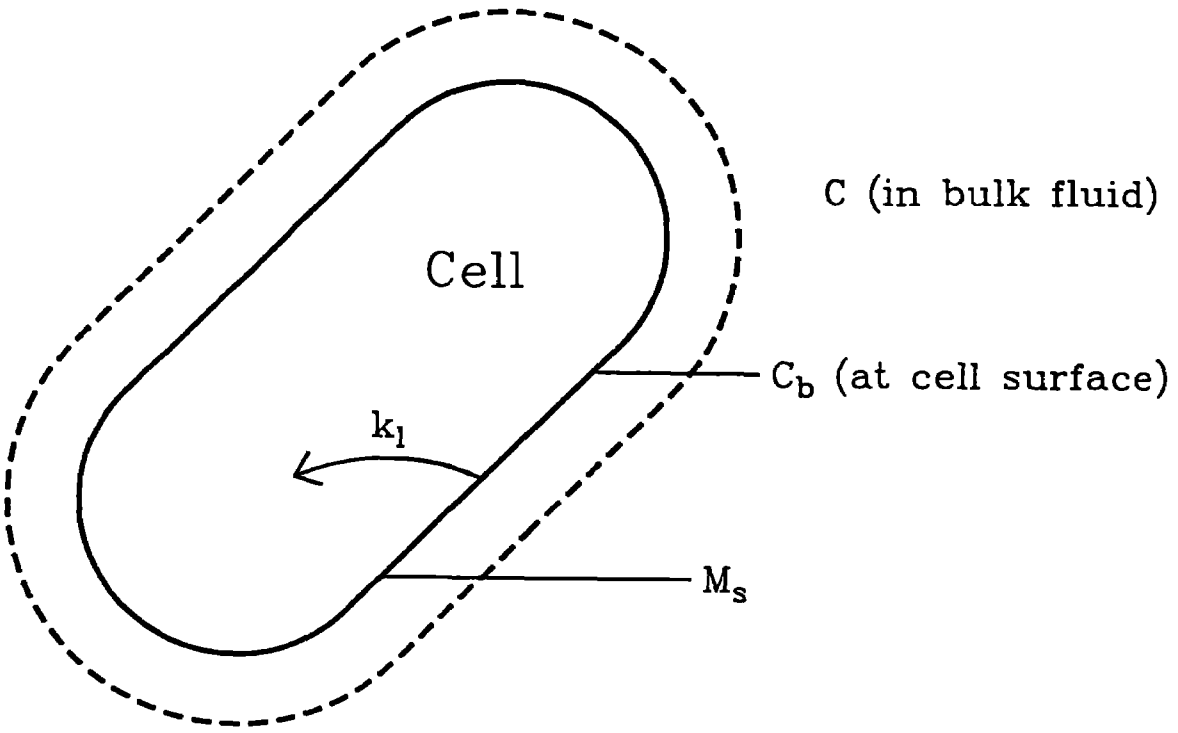

Figure 4. Diagram of Cell in aquatic medium indicating the concentration gradient surrounding the cell.

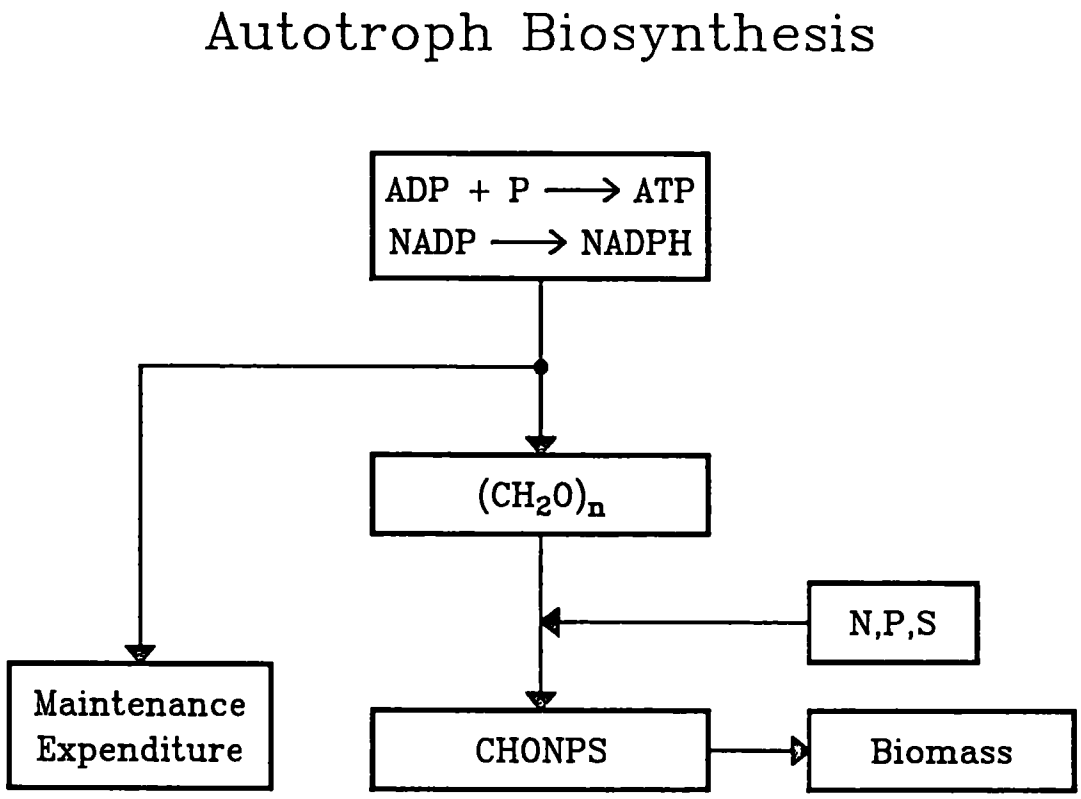

Figure 5. Major components and relationship of autotroph biosynthesis.

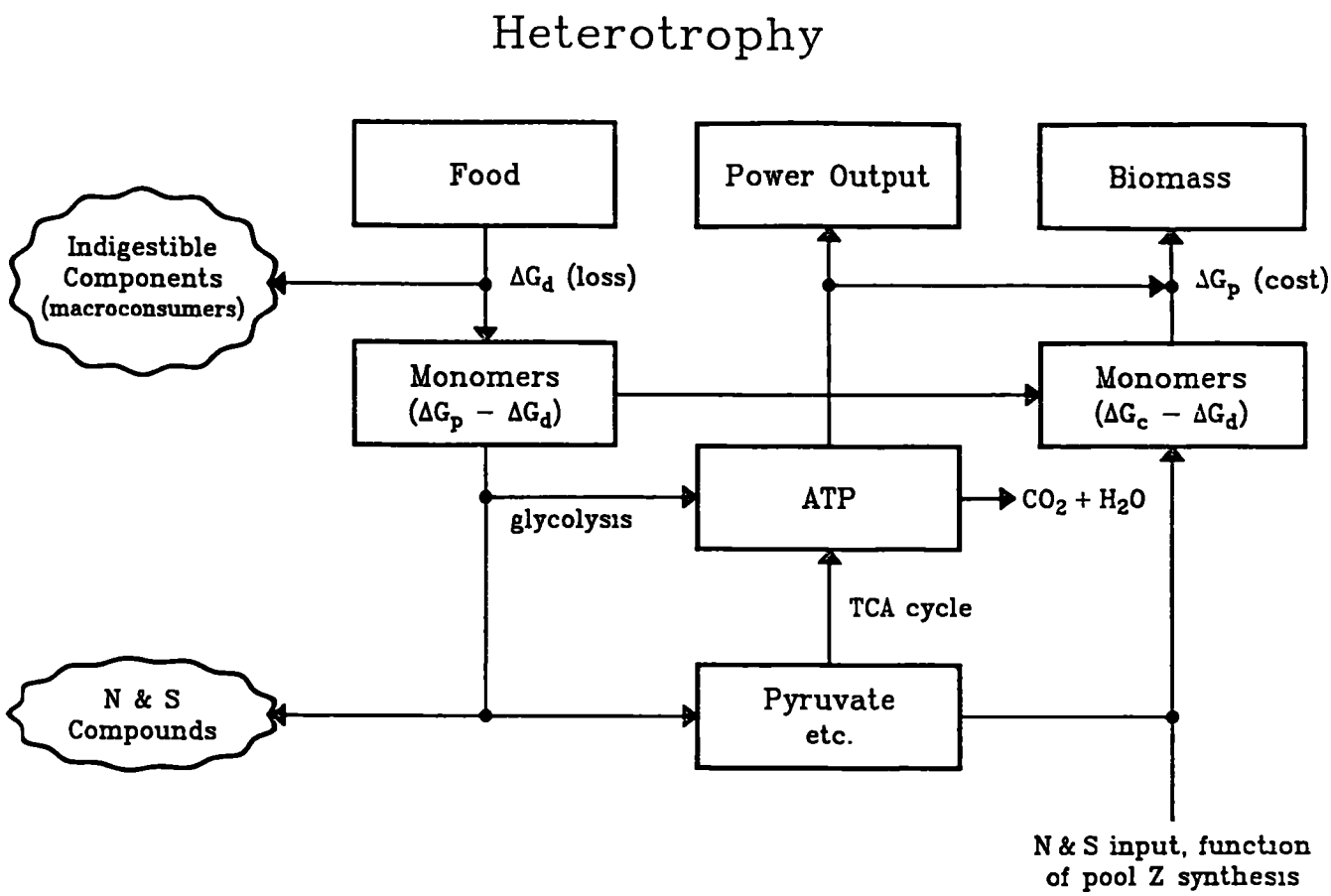

Figure 6. Major components and pathways (energy and mass) of heterotrophy.

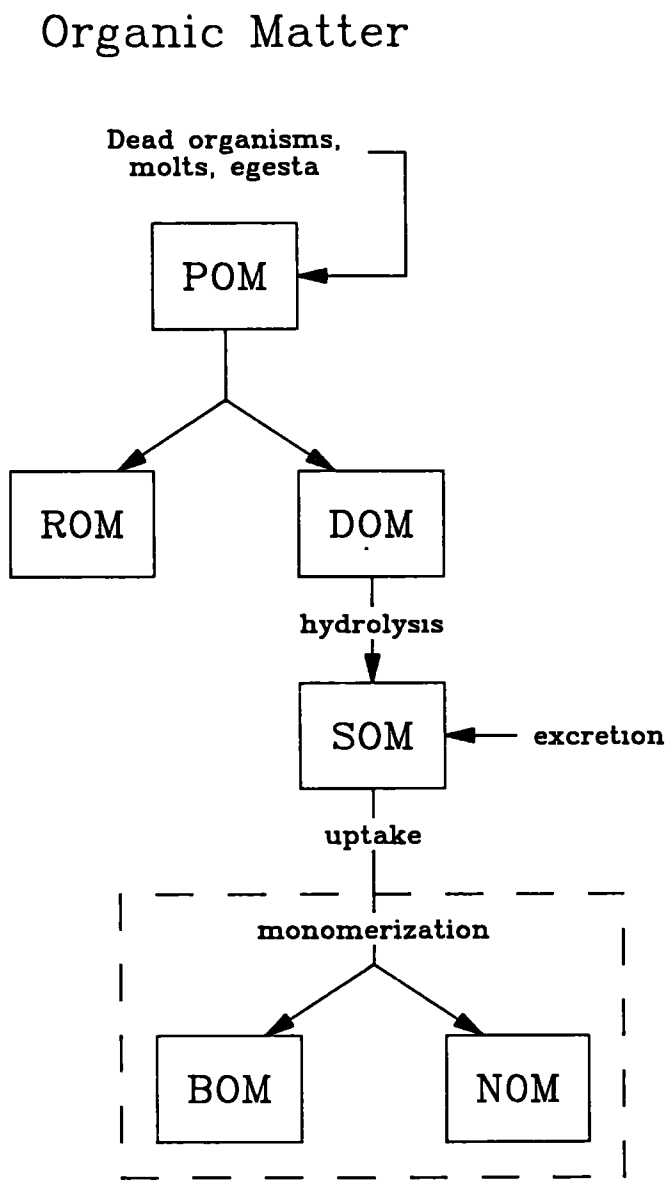

Figure 7. Categories of organic chemicals (P=particulate, R=refractory, D=digestible, S=soluble, B=biomass-like, N=non-biomass-like)

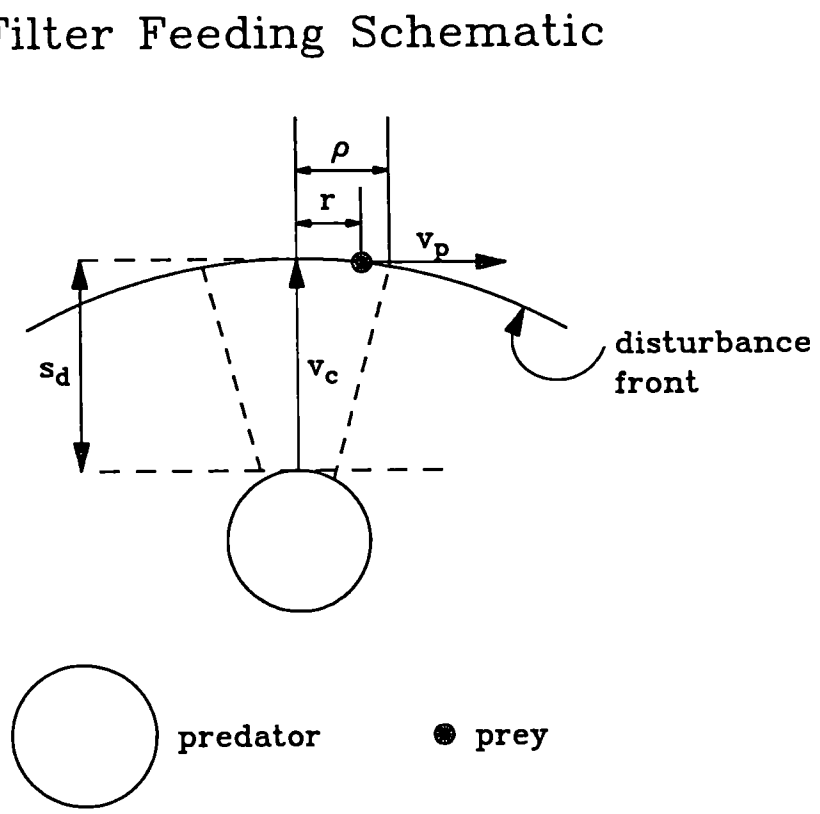

Figure 8. Relationships characteristics of a filter feeding predator and its potential prey that determine probability of capture.

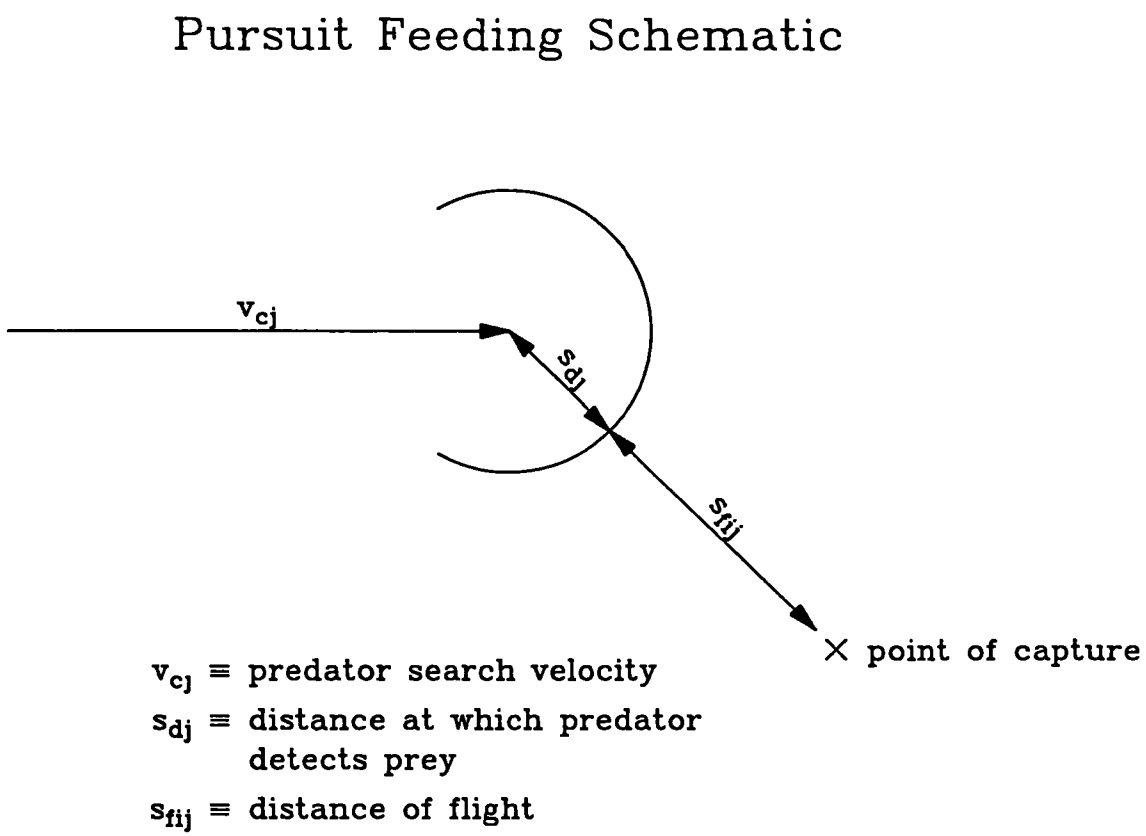

Figure 9. Relationships between characteristics of a pursuing predator and its potential prey.

Table 1

Some reactions used by chemoautotrophs for energy

Reaction	Free Energy kcal/M(substrate)	kcal/eq.wt.(substrate)
$NH_4^+ + 1.5\ O_2 = NO_2^- + 2\ H^+ + H_2O$	-64.92	-10.82
$NO_2^- + .5\ O_2 = NO_3^-$	-18.50	-9.25
$HS^- + 2\ O_2 = SO_4^{2-} + H^+$	-190.30	-23.79
$S^0 + 5/2\ O_2 + H_2O = SO_4^{2-} + H^+$	-139.98	-23.33
$S_2O_3 + 2\ O_2 + H_2O = 2\ SO_4^{2-} + 2\ H^+$	-190.16	-23.77
$SO_3^{2-} + 1/2\ O_2 = SO_4^{2-}$	-29.54	-29.27
$HS^- + 8/5\ NO_3^- + 3/5\ H^+ = SO_4^{2-} + 4/5\ N_2 + 4/5\ H_2O$	-177.92	-22.24
$S^0 + 6/5\ NO_3^- + 2/5\ H_2O = SO_4^{2-} + 3/5\ N_2 + 4/5\ H^+$	-130.74	-21.79
$\cdot_2 + 2/5\ NO_3 + 2/5\ H^+ = 1/5\ N_2 + 6/5\ H_2O$	-53.60	-26.80
$H_2 + 1/4\ SO_4^{2-} + 1/4\ H^+ = HS^- + H_2O$	-9.10	-4.55
$H_2 + 1/2\ CO_2 = CH_3COOH + 1/2\ H_2O$	-4.30	-2.15
$CH_4 + 2\ O_2 = CO_2 + 2\ H_2O$	-195.50	-24.44
$CH_4 + SO_4^{2-} + H^+ = CO_2 + HS^- + H_2O$	-5.20	-0.65

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16. ABSTRACT

A strategy is developed for modeling ecosystems to permit assessment of effects of toxic chemicals on element cycling and other ecosystem processes. The strategy includes use of multi-species representations of biotic communities and mathematical descriptions of the processes that are important in aquatic ecosystems. Direct effects of toxicants are assigned to the species comprising the biotic community in a manner suggested by available toxicological information. Effects are calculated as the difference between selected measures of processes from unaffected systems and systems affected by the presence of a toxic chemical. Ecological effects calculated in this manner are considered to be heuristically useful.

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