United States Environmental Protection Agency
Research and Development
Environmental Research Laboratory Athens GA 30613
EPA-600/S3-83-084 Nov. 1983

EPA

Project Summary

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

Ray R. Lassiter

A strategy was developed for modeling ecosystems to permit the assessment of toxic chemical effects on element cycling and other ecosystem processes. The strategy includes the 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.

This Project Summary was developed by EPA's Environmental Research Laboratory, Athens, GA, to announce key findings of the research project that is fully documented in a separate report of the same title (see Project Report ordering information at back).

Introduction

Analysis of environmental risks posed by the release of toxic chemicals necessarily would require predictions of the fate of a chemical and its effects. Prediction of a chemical's fate presupposes an understanding of transport and transformation processes, or "what the environment does to the chemical." Prediction of a chemical's effects presupposes a wider knowledge of the chemical's fate, and by contrast, "what the chemical does to the environment." It is also necessary to know which effects are of concern, because very many potential effects exist. Ecological effects are the concern of this research, and effects that occur in ecosystems, and whose characteristics are influenced by ecological interactions, are considered to be ecological effects. A particular class of potential ecological effects that arguably could be of major significance are effects on cycles of elements. Although results of this research will not be limited to consideration of the effects of toxicants on element cycles, they are the class of effects that have motivated most of the work. A major reason for focusing on element cycle effects is that there is apparently no ongoing work in this area despite the apparent potential for such effects.

The Nature of Element Cycles and Importance of Considering Their Response to Toxicants

Biotic processes in the proportions and magnitudes that we know them depend upon concentrations of chemicals remaining approximately at their current levels. The energy for biotic processes is derived from catalysis of redox reactions between reduced and oxidized forms of elements. The primary source of the disequalibria that drive these reactions is photosynthesis in which both highly reduced organic compounds and molecular oxygen are produced. The remaining biotic processes feed off this disequilibrium, and in doing so contribute to maintenance of the pool sizes of geochemicals. These include the atmospheric gases, the composition of the ocean, dissolved constituents of fresh waters, and the earth's soils.

These geochemical pools have been remarkably stable over geological time scales. This fact attests to the historical stability of the contributory processes. No comparative analysis of the relative roles of abiotic and biotic processes in maintaining the pools of geochemicals has been made. The number and importance of the processes known to be carried out by organisms, however, leaves little doubt that the characteristics of the earth depend on the continuation of biotic processes at about their current levels. Whether these processes will remain stable in the presence of continued introduction of xenobiotic chemicals is unknown. It is prudent, therefore, to consider potential conditions that could lead to serious disturbances of element cycle transformations. Conditions that would lead to alterations in ecosystem structure and function are expected to lead to corresponding alterations in element cycling.

Strategy of Ecosystem Modeling for Analyzing Alterations in Element Cycling

Element cycling is a system phenomenon. Organisms use pools of chemicals that are products of other organisms' metabolism. These and other phenomena that occur as fluxes that change chemical forms and redox states are processes. For a given set of elements one can describe the major processes that occur to cycle the elements through their various forms. They can be grouped into those pertaining to microrganisms or macroorganisms and to autotrophs or heterotrophs. The level of resolution at which these processes are described is a critical choice for accomplishing the desired goals. These goals are to represent the aquatic ecosystem such that models of the processes respond to external influences, including the introduction of toxicants approximately the same as do real systems. If this goal is reached, it will be possible to analyze for ecological effects of toxic chemicals, including their effects on element cycling processes. Carrying out analyses of this sort is, in a special sense, a predictive (or prognostic) exercise that is fully comprehensible only if the usage of the term "effect" is understood, and if the special sense of prediction is made clear.

An effect implies a deviation from some nominal state or rate. In this model, therefore, the effect is referred to as a deviation from a nominal condition. This deviation can be obtained by first using the model to obtain the nominal condition, then using it again in the same manner, but with the presence of a toxicant represented additionally. To normalize effects so that measurement units do not influence the magnitude of the values, the difference should be divided by the nominal value. Any quantity of interest can be used to calculate an effect, from the amount of a material present to the rate at which a process is occurring, regardless of whether there is any direct influence of the toxicant on the quantity of interest. Because the effect is obtained by model calculation in which comparable conditions can be strictly maintained, and it is known that the only difference between the nominal and affected conditions is the presence of the chemical, any differences can be attributed to the presence of the chemical and referred to, therefore, as an effect. These calculations are referred to as predictions of ecological effect of the toxic chemical.

The special sense in which "predictions" is used is that the predicted values have heuristic value but do not refer to an expected effect in a particular real ecosystem at some time. The predicted value is intended to be heuristically useful by permitting assessment of the probable effects in aquatic ecosystems of selected characteristics without necessarily referencing specific real aquatic systems. The strategy of modeling is designed to make this use possible.

The strategy of modeling makes use of representation of multiple species, each carrying out a particular process. It is often observed that concentrations of environmental chemicals that are known to turn over rapidly are fairly stable, whereas any particular species that uses or produces the chemical may fluctuate widely. This suggests that compensation occurs among species carrying out the same function. That is, reduction in levels of one species may be compensated by corresponding increases in the levels of one or more others, so that the processes responsible for the level of the chemical are relatively stable. The possibility of stability resulting from species redundancy and compensation is important when considering the effects of chemicals on the cycling of major elements. If this phenomenon is important, it is probable that representing a group of organisms by a single variable (as opposed to a multi-species representation) would lead to conclusions that element cycling processes are more fragile than they. in fact, are.

Another important component in this modeling strategy is the way that element cycling processes are represented by species populations. In element cycling, it is the processes that are important. They are carried out, however, by particular populations. Each individual species population is characterized by size, energy source, source of materials for biosynthesis, motility, and several other descriptors. The descriptors will define a particular population as carrying out a specific process. Representations of multi-species populations will differ among themselves in the particular values of the descriptors. For example, one population may consist of large individuals that move slowly and use biomass of microorganisms for both energy and biosynthesis, while another may differ in being smaller and moving more rapidly. These organisms are represented differently from carrying out different processes by differences in the energy source and source of materials for biosynthesis. For example, another group of organisms might use NH_4^+ and O_2 for energy and inorganic chemicals for biosynthesis.

Representing the organisms that exist in systems to carry out all the important functions using this approach requires that a large amount of descriptive data be available. That amount of data will not be available for all the organisms necessary to represent the processes of any given ecosystem. Therefore, the use of this approach requires an additional strategic component to make it possible to parameterize the model for the large number of species representations necessary to the approach. Essentially this will be accomplished by first describing a large number of species for the initial set of organisms that occupy the environment. Selection of the descriptors will be guided by what is known about the kinds of organisms carrying out the various ecosystem processes, *i. e.,* they will be assigned to the model representations over a range that includes what is known. It is unlikely that an assignment can be made such that the entire initial set will persist for very long (not approach zero).

It is anticipated, however, that some of the variables will be persistent. These will represent a set of organisms that are inter-compatible and that are "adapted" to the environment. It is extremely unlikely that this set will well represent real populations (in the sense of close correspondence of their descriptors to those of real populations). Yet, their descriptors necessarily will be in the neighborhood of those of real populations, because only such descriptors are to be used. Repeated selection of compatible sets of organism representations for a given environment beginning with different initial sets is expected to build a distribution of descriptors that would include the characteristics of real organisms that would live in the environment as described.

This synthetic approach appears to be the best way to obtain descriptions of biotic communities that are appropriate for an environment that is selected for assessment in anticipation of a toxic chemical's possible introduction. With this approach a nominal behavior of element cycling processes can be obtained. The same type of uncertainty exists for the direct effects of a toxic chemical on the organisms of a community, however, as exists for the characteristics of types of organisms that inhabit the community. The final element of the strategy defines the process by which toxicological information is used to obtain affected behavior.

For each set of compatible species representations, a set of direct effects will be assigned from the range of direct effects suggested by the available toxicological information. Recalculation of the behavior in the presence of the toxicant, then, will build another distribution of behaviors. Normalized differences between the two behaviors, as already discussed, are the ecological effects of the chemical.

It is readily apparent that ecological effects calculated in this manner are not expected to be observed exactly in any particular system. They are expected, however, to include values for real systems similar to the one analyzed. Furthermore, if the nature of the distribution of descriptors of the compatible sets of species and of the direct effects of toxicants on them is realistic, a measure of the uncertainty associated with the predicted effects can be obtained. The value of the calculated effects will not be primarily quantitative, however, but rather, will more appropriately be used as a learning exercise for identification of possible ecological effects that are too far removed from the direct effects to be apparent without an ecosystem model.

Descriptions of the Processes

Much of the research effort was devoted to assimilation of existing and development of new mathematical descriptions of the processes. Uptake of materials by microorganisms is described by a rectangle hyperbola that is derived in a way that rationalizes its use for all uptake processes. Depletion of materials being taken up from a zone in the vicinity of cells is considered. Photoautotrophy is described in terms of both bioenergetics and uptake of materials, so that limitation by light and materials is possible. Chemoautotrophs and photoautotrophs share the same biosynthetic pathways. Chemoautotrophs, however, use a variety of terminal electron acceptors. The bioenergetics of their energy reactions is used to calculate the rate of energy production, and as with photoautotrophs and for that matter all organisms, limitation of growth is considered to be the minimum of the potential growth rates for each of the requirements. Photoautotrophs produce organic matter using solar energy, whereas, chemoautotrophs produce organic matter using energy of redox reactions between reduced forms of inorganic compounds and oxygen. In the process, oxidized forms of elements are formed. The reduced forms of the inorganic compounds are produced by heterotrophs using oxidized species of elements in anaerobic zones.

Heterotrophic processes are represented for both microorganisms and macroorganisms. All use organic compounds for both energy and for synthesis. Microorganisms are found in both aerobic and anaerobic zones of aquatic systems. In aerobic zones they use molecular oxygen as their terminal electron acceptor (oxidizing agent) for oxidizing organic compounds. In anaerobic zones oxidized forms of the major elements are used as terminal electron acceptors. These oxidized forms are those produced by chemoautotrophy. In this manner, the element cycles are completed. Growth of heterotrophs is described as the difference between the available energy and materials and their need for maintenance and activity. Macroheterotrophs differ from microheterotrophs in being limited to aerobic environments and in their use of specific structures and behaviors to obtain food. Two major kinds of feeding are described for the model: filter feeding and pursuit feeding. General model descriptions for both types are developed for the general case of any number of consumers feeding on any number of prey. Rates of consumption are calculated directly from characteristics of predator and prey, rather than assigned as coupling constants.

Outlook

The strategy of modeling and the requisite theory to carry it out exist. Additional work is needed to bring the expression of toxicological theory to the state of development (in the context of this model) as the theory for ecosystem modeling. Further work is needed to represent fermentation as an ecological process. Coding is underway for the ecosystem model. Whether the sets of compatible representations of biotic communities and the effects as computed will be usefully close to real systems needs to be tested. The fact that no specific real system is represented presents a difficulty in that regard. Laboratory ecosystems, however, can be run repeatedly under the same conditions and with or without the presence of a toxicant. One potential testing scheme would make use of this capability and compare distributions and effects from laboratory ecosystems with distributions and effects from the model as described.

*The Project Summary was authored by **Ray R. Lassiter** who is also the EPA Project Officer (see below).*

The complete report, entitled "Prediction of Ecological Effects of Toxic Chemicals: Overall Strategy and Theoretical Basis for the Ecosystem Model," (Order No. PB 83-261 685; Cost: $10.00, subject to change) will be available only from:
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
Telephone: 703-487-4650

The EPA Project Officer can be contacted at:
Environmental Research Laboratory
U.S. Environmental Protection Agency
Athens, GA 30613

☆ U.S. GOVERNMENT PRINTING OFFICE: 1983—659-017/7227