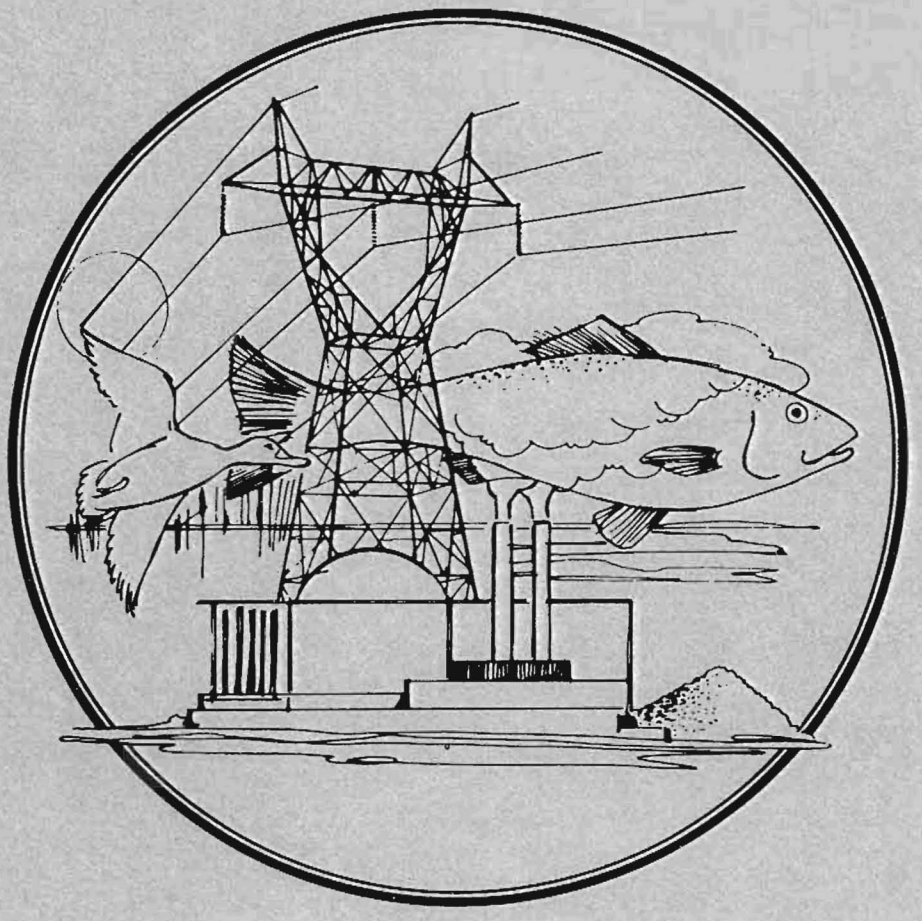
Biological Services Program

FWS/OBS-80/40.12
July 1982

Air Pollution and Acid Rain,
Report No. 12

Effects of Acid Precipitation on Aquatic Resources: Results of Modeling Workshops



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EFFECTS OF ACID PRECIPITATION ON AQUATIC RESOURCES: RESULTS OF MODELING WORKSHOPS

Project Officer

R. Kent Schreiber
Eastern Energy and Land Use Team
Route 3, Box 44
Kearneysville, WV 25430

Cooperatively Produced By

by

Eastern Energy and Land Use Team
Route 3, Box 44
Kearneysville, WV 25430

and

Western Energy and Land Use Team
Creekside One, 2625 Redwing Road
Fort Collins, CO 80526

Fish and Wildlife Service

U.S. Department of the Interior

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For additional information on this report, or the workshops, contact:

Orie Loucks
Science Director, The Institute of Ecology
4600 Sunset Blvd.
Indianapolis, IN 46208

Kent Schreiber
National Power Development Group
(formerly National Power Plant Team)
Eastern Energy and Land Use Team
U.S. Fish and Wildlife Service
Route 3, Box 44
Kearneysville, WV 25430

Richard Ellison
Leader, Adaptive Environmental Assessment Group
Western Energy and Land Use Team
U.S. Fish and Wildlife Service
2625 Redwing Road
Fort Collins, CO 80526

EXECUTIVE SUMMARY

The United States discharges approximately 50 million metric tons of sulfur and nitrogen oxides into the atmosphere annually. These pollutants, following atmospheric transport, impact a broad geographical area. The pattern of increasing acidity and decreasing biological productivity now being noted in poorly buffered lakes in the northeastern United States coincides both in time and place with the pattern of rainfall acidity (Tennessee Valley Authority 1980). Areas affected by acid precipitation appear to be expanding southward and westward, and recent evidence points to increasing problems with acid rain on the West Coast (Powers and Rambo 1980).

The passage of the Clean Air Act of 1963 (Public Law 88-206, 77 Stat. 392) and its 1977 Amendments (Public Law 95-95, 91 Stat. 731) resulted in a number of regulations designed to protect air quality. Incorporated into this legislation was a new responsibility for Federal land managers, including the Fish and Wildlife Service (FWS), to assess impacts of air quality degradation on related values for lands under their jurisdiction (Avery and Schreiber 1979). The FWS, along with other Federal and State agencies, needs comprehensive, current information on the ecological effects of air pollution, including acidic precipitation, in order to meet this responsibility.

In response to this information need, the FWS initiated an air pollution and acid rain program to determine the magnitude of the problem, the nature and extent of damage to terrestrial and aquatic biota, and possible mitigation measures and to develop an information base that regulatory agencies can use in the formulation of their policy. However, major gaps were found to exist in the essential information needed for these assessments. In addition, existing research results were scattered and often difficult to interpret in terms of the needs of FWS biologists. It became apparent that better organization of current knowledge and identification of critical research needs in relation to acid precipitation impacts on fish and wildlife resources was needed.

In response to these needs, the FWS National Power Development Group (NPDG) sponsored a series of Adaptive Environmental Assessment (AEA) workshops on acid precipitation. The objectives of these workshops were to:

(1) encourage communication among scientists studying various phenomena related to acid precipitation;

(2) develop a framework for integrating existing information; and

(3) identify priority research needed for a better understanding of the acidification process and its impacts on aquatic resources of watershed ecosystems.

The first workshop, facilitated by the AEA Group of the Western Energy and Land Use Team (WELUT), FWS, was held in August, 1980, in Ann Arbor, Michigan. Approximately 30 scientists studying the acid rain problem participated in the 5-day workshop. This workshop was too short to address fully the objective of establishing research priorities for so complex a subject as acid precipitation effects on aquatic resources. However, participants did initiate an assessment of research needs (Andrews et al. 1980); the assessment was continued at subsequent workshops.

Because the resource systems in question are very complex, the initial workshop was structured around the conceptualization and parameterization of a computer simulation model that could be used to describe and integrate the mechanisms by which acid precipitation alters stream and lake chemistry and impacts fish populations and other aquatic components. Four submodels were developed in order to examine the relationships and research needs among the linked components of terrestrial and aquatic systems: (1) the watershed system, which receives input from the atmosphere and yields chemically altered surface and ground waters; (2) changes in the chemistry of aquatic environments, particularly relatively infrequent abrupt pH depressions; (3) food chain components, including algae, zooplankton, and benthic organisms, some of which are themselves sensitive to low pH; and 4) key fishery populations.

Three subsequent workshops were held in Fort Collins, Colorado, in March, May, and August, 1981, to review, evaluate, and refine the preliminary model.

Watershed data bases from Harp Lake in Ontario and Filson Creek in Minnesota were available for partial model calibration, evaluation of model output, and identification of research needs.

The primary research need identified during the acid precipitation workshops was integrated watershed studies that include major abiotic and biotic components. Studies that are comprehensive enough to provide all the data necessary for parameterizing and validating this or similar models have not been conducted. Aquatic biota usually are not considered when selecting calibrated watersheds for ecosystem level studies. Criteria and biotic information which should be assessed, along with physical features, when selecting sites for calibrated watershed studies include: a fish community that is representative of species in the region; the ability to control or measure human use of the fishery; the ability to control or measure emigration and immigration of the fish populations; and the ability to monitor lower trophic levels on a seasonal basis. This type of integrated watershed data base is essential if we are to develop a better understanding of the effects of acid precipitation on aquatic resources and refine and validate models enough to address management concerns with confidence.

Additional research needs and model limitations identified during the acid precipitation workshops were related to specific aspects of model conceptualization and parameterization. Major information needs associated with the watershed submodel include: (1) the nature of acid deposition (e.g., relative amounts of SO_x and NO_x and distribution of acid inputs between dry, gaseous, and wet forms); (2) factors which determine susceptibility of a watershed to acidic inputs; (3) the nature and kinetics of important chemical reactions in the soil profile, including leaching and exchange of metals and metaloids, due to precipitation of different amounts and pH; (4) terrestrial biological modifications of acidic inputs and their influence on lake acidification; and (5) the influence of ground water on lake acidification. Key water chemistry needs include: (1) the influence of hydrogen ions and ligands, such as fluoride and organic acids, on aluminum chemistry in dilute water systems; (2) the speciation and ligand associations of potentially toxic trace metals; (3) the importance of sediments in modifying buffering capacity and toxicity of metal forms in dilute water systems; and (4) spatial differences in acidification

and dilute water chemistry associated with lake stratification. Important information needs with regard to lower aquatic trophic levels include: (1) influence of acidity on species diversity and community composition; (2) effect of acidity on the cycling of phosphorous, which is limiting in many aquatic systems; and (3) the direct and indirect influences of acidification on photosynthetic capacity and food chain energetics. Primary information needs associated with fisheries include: (1) effects of acidity on bioenergetics (e.g., partitioning of energy for growth, reproduction, and metabolism) and secondary consequences related to food chain energy transfers; (2) determination of the relationship between pH-aluminum levels and fish mortality for species other than brook trout and white sucker; (3) development of pH-related mortality functions for metals such as copper and zinc, which may be of greater importance than aluminum in some geographical areas; (4) chronic effects of acidification (e.g., inhibition of gametogenesis); and (5) potential compensatory responses of fish to acidification.

The simulation model developed during this project was not intended to be a predictive management tool and, at its current level of refinement, use of the model for predictive purposes is inappropriate. Rather, the process of building and testing the model was used to: (1) provide a framework for identifying research and model refinements needed in order to adequately address the effects of acid precipitation on aquatic resources; and (2) develop a more holistic understanding of the acidification process and its consequences.

When the problem of acid precipitation is considered from a holistic viewpoint, it becomes obvious that fishery resources are only a subset of the interconnected biotic and abiotic components of a watershed ecosystem. Consequently, questions about the effects of acid precipitation on fish resources, which FWS biologists must increasingly address, require an interdisciplinary, holistic approach to the problem. It is recommended, therefore, that the FWS develop a fish and wildlife research strategy that will ensure that these interdisciplinary links are recognized and addressed.

As our understanding of the acidification process and biological responses to the process increases, models can be built that will more accurately represent the important interactions. As a result, these simulation models could be used predictively to trace the effects of acid precipitation through a watershed ecosystem and to address potential management strategies. Models, however, will remain incomplete representations of real world systems and, as such, should be only one of the tools used to make management decisions.

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1. INTRODUCTION

SCOPE AND GOALS

The passage of the Clean Air Act of 1963 (Public Law 88-206, 77 Stat. 392), and its 1977 Amendments (Public Law 95-95, 91 Stat. 731), resulted in a number of regulations designed to protect air quality. Incorporated into this legislation was a new responsibility for Federal land managers, including the Fish and Wildlife Service (FWS), to assess the impacts of the degradation of air quality on related values for lands under their jurisdiction (Avery and Schreiber 1979). The FWS, along with other Federal and State agencies, needs comprehensive, current information on the ecological effects of air pollution, including acidic precipitation, in order to meet this responsibility. The series of simulation modeling workshops described in this report were conducted to identify and document critical information gaps related to long term alteration of aquatic ecosystems.

President Carter's environmental message to Congress in August 1979 stated that acid rain was second only to increased carbon dioxide levels as the most serious threat to the environment. The President directed the reprogramming of $10 million per year into acid rain research and the creation of a Federal Acid Rain Assessment Program. The FWS has included acid precipitation high on its list of priorities in terms of the Nation's Important Resource Problems (IRP's).

An Interagency Task Force completed the National Acid Precipitation Assessment Plan in 1980 (Council on Environmental Quality 1981). This plan outlines a program in which Federal agencies would cooperate in research and assessment relating to the production, transport, deposition, and effects of acidic or acid-forming substances. One section of the plan discusses research needs related to the effects of acid rain on aquatic ecosystems. The potential contributions of a number of Federal agencies with resource responsibilities for soil, water quality, and biological components to resolving these problems are described. The Environmental Protection Agency (EPA) was given the lead

responsibility for coordination of work concerning aquatic effects. The Department of Interior is involved in several subcomponent areas, particularly modeling and assessment of effects of acid precipitation on stream and lake ecosystems. Within the Department of Interior, the FWS, through its Division of Research and Office of Biological Services, has programs and personnel involved in the assessment of the effects of acid rain on fish, wildlife, and their habitats.

The international implications of acidic rainfall were recognized in 1980 when the United States and Canada signed a Memorandum of Intent (MOI) committing both countries to examine the sources and consequences of transboundary pollutants. Four Work Groups were established in late 1980, one of which was to address the aquatic, terrestrial, material, and health effects of transboundary pollutants. A preliminary report from this Work Group in early 1981 (Anonymous 1981) indicated that the major bi-National concern would probably focus on aquatic effects of acidic deposition. An overview of the mechanisms involved that can be incorporated into a simulation model, such as the one described in this report, is expected to be an important contribution to the U.S./Canadian studies, as well as to the definition of research needs in the EPA and FWS programs.

The National Acid Precipitation Assessment Plan and the recent work done cooperatively by the United States and Canada (Anonymous 1981) indicate that acid rain is becoming widely recognized as a problem that may require new legislative and regulatory initiatives. Sound biological information on the ecological effects of acid rain, including projections of acid precipitation trends are prerequisites to effective legislation. The resolution of problems associated with acid rain depends on a thorough understanding of the sources of acidic pollution, its transport and deposition, its impact on aquatic and terrestrial ecosystems, and the development of cost effective mitigation measures.

OVERVIEW OF THE PROBLEM

The United States discharges approximately 50 million metric tons of sulfur and nitrogen oxides into the atmosphere annually. These pollutants, following atmospheric transport, impact a broad geographical area. The pattern of increasing acidity and decreasing biological productivity now being noted in poorly buffered lakes in the northeastern United States coincides both in time and place with the pattern of rainfall acidity (Tennessee Valley Authority 1980). Areas affected by acid precipitation appear to be expanding southward and westward, and recent evidence points to increasing problems with acid rain on the West Coast (Powers and Rambo 1980).

Rainfall is naturally slightly acidic, due to its carbon dioxide content. Rain can be further acidified from the chemical conversion of atmospheric sulfur and nitrogen compounds, by-products of fossil fuel combustion, or hydrochloric acid resulting from the combustion of coals containing chlorine. Sulfur oxides, which are usually only a small percentage of the air pollutant load at most locations, apparently are responsible for approximately 60% of the acidity of rain in the eastern United States. Nitrogen oxides account for most of the remaining acidity. The ways in which oxidation and subsequent acidification of rain can occur are complicated and depend on a number of factors, including the intensity of sunlight, heavy metal concentrations, and the amount of ammonia present.

Research programs, for the most part, have emphasized how the acidification process takes place, including atmospheric tranformations and biogeochemical alterations in terrestrial and aquatic systems (Council on Environmental Quality 1981). Most studies of the effects of acid precipitation on biota have been short term laboratory investigations and synoptic field surveys. Comprehensive studies of how acid precipitation stress on an organism translates into effects on the population and community have not been conducted.

The possible interactions within an aquatic ecosystem are complex and cannot easily be described. For example, existing information indicates that the acid neutralizing capacity of aquatic systems has been reduced by the elevated acidity of input water. Once the acid neutralizing capacity is

reduced, pH can decline rapidly, triggering a series of ecological and geochemical changes. For example, a high concentration of hydrogen ions in the water may increase the rate of release of toxic trace metals, which would otherwise remain in the soil or in lake bottom sediments (Gorham 1976; Dvorak and Lewis 1978). The increased amount of these metals may adversely affect fish and other aquatic biota. Consequently, an interdisciplinary conceptual framework for the organization of existing laboratory and field research results on acid precipitation is needed.

U.S. FISH AND WILDLIFE SERVICE INFORMATION NEEDS

Acid rain is a major concern of the FWS because of its potential for damaging the biota in both terrestrial and aquatic ecosystems. The FWS has, therefore, initiated an air pollution and acid rain program to help determine the magnitude of the problem, the extent of damage, biological consequences, and possible methods of mitigation, as well as to develop an information base that can be used by regulatory agencies in the formulation of their policy.

Acid precipitation can impact aquatic ecosystems, and fish resources specifically, in numerous ways (Fromm 1980; Fritz 1980). There are several programs investigating the impact of acidic precipitation on aquatic ecosystems (e.g., EPA-Duluth, Electric Power Research Institute (EPRI), North Carolina State-EPA, FWS, and numerous State agencies), each with a particular objective in mind. Fish and Wildlife Service biologists are likely to become increasingly involved in assessing the potential impacts of acid precipitation on fish and wildlife resources. However, major gaps in essential information exist for these assessments. Existing research results are scattered and may be conflicting or even uninterpretable in terms of the particular needs of FWS biologists. It is apparent that a better organization of current knowledge is needed and that, by building on that knowledge, critical data needs in relation to impacts of acid precipitation on fish and wildlife resources can be identified.

The FWS National Power Development Group (NPDG, formerly the National Power Plant Team) sponsored a series of workshops involving approximately 40 invited participants in order to identify critical information needed to assess the impacts of acid rain on aquatic resources. The workshops focused on the types of research that would specifically address long term responses in the complex of factors that influence fish and wildlife resources. The multidisciplinary group included scientists and technical experts from a variety of research programs currently investigating the acid rain problem, as well as research managers and policymakers.

The workshops provided an atmosphere where scientists could develop a framework for considering the mechanisms of acid rain impacts on aquatic resources and define priority research needs related to the effects of acid rain on fish resources in freshwater lakes. Systems of interest included oligotrophic cold water lakes and streams in the northeastern and northcentral United States. The geographical areas selected reflect the current information base, rather than a bias for any particular location. Simulation modeling of a watershed/lake ecosystem was used to facilitate communication among the workshop participants and to improve the understanding of the problem through preliminary analysis of the quantitative linkages within the system. The workshops and the synthesis process were facilitated by the Adaptive Environmental Assessment (AEA) Group of the U.S. Fish and Wildlife Service.

2. THE WORKSHOP MODELING APPROACH

Adaptive Environmental Assessment modeling (Holling 1978) involves decisionmakers, planners, scientists, and other interested parties in highly structured workshops that focus on information needs for the decision process. Workshops are structured around the construction and refinement of a simulation model of the resource system under consideration; in this case, the consequences of acid deposition on aquatic resources. The process of constructing the model helps specify the relative importance of each model component in determining system response; these differences in importance are ued in the identification of research needs. The limited time available during a workshop prevents the subdivision of problems into increasingly finer detail; judgements must be made concerning what can be realistically incorporated into the analysis. Managers and administrators become familiar with the basic assumptions and limitations of the analytical techniques being used. They also provide the practical focus necessary to keep the analysis relevant to management and decisionmaking issues. In addition, all participants are challenged to communicate their ideas about how the resource system functions clearly and concisely. Effective communication is essential in clarifying points of agreement and contention, identifying data gaps, and evaluating research priorities.

WORKSHOP STAFF AND ACTIVITIES

Modeling workshops, in the Adaptive Environmental Assessment process, are facilitated by a staff trained in systems analysis, computer modeling, policy analysis, and group dynamics. The staff has four primary functions during the course of a workshop: (1) to moderate the workshop; (2) to help participants construct a computerized simulation model of the resource system under consideration; (3) to help participants interpret model output; and (4) to aid in the integration of workshop results into relevant research and management activities.

The first activity in a modeling workshop is defining the problem and the space, time, and scientific bounds of the problem. Considerable effort is devoted to identifying the quantities (indicators) that describe the resource system and the actions or societal demands that management must consider. The resource system is usually divided into a number of logical components for detailed consideration by subgroups. Before breaking into subgroups, the participants define how the components of the resource system interact. This interdisciplinary exercise helps the participants understand the entire resource system and becomes the basis for building a simulation model and developing alternative management action scenarios later in the workshop.

Participants divide into small working subgroups according to their areas of expertise and interest. Subgroup meetings are convened by members of the workshop staff. Each subgroup defines and tries to quantify the functional relationships that describe the behavior of the component they are considering with respect to the resource system as a whole. The subgroup utilizes both the indicators and management actions and the interactions between resource system components identified earlier in the workshop.

Once the submodels developed by the subgroups have been programmed by the staff, the process of model evaluation begins. Model evaluation in the acid rain workshops focused on additional research needs. Evaluation involves examining the response of the model to various management scenarios. Even more importantly, information needed for the model in order to have confidence in the ability of the model to predict system responses can be explicitly identified. Participants may suggest appropriate changes in data or functional relationships as a result of the model evaluation. The workshop staff tries to incorporate these changes into the model, although additional data may be needed. Management scenarios are rerun to examine the implications for all interest groups involved. The resulting model represents a group concensus concerning assumptions and general resource behavior, and the research needs identified provide a strategy for improving the understanding and predictive potential of the model. Although the initial model is not necessarily scientifically precise, it represents the group's best estimate of how the resource

system functions. This group perspective is usually superior to that of any one individual. Subsequent technical meetings and workshops may be held in order to refine and analyze the model.

EXPECTATIONS FROM AEA WORKSHOPS

The AEA workshop process is an exercise in interdisciplinary modeling and can contribute to several aspects of environmental assessment, including those discussed below.

Interdisciplinary Communication and Public Participation

Scientists and policymakers from Federal, State, and local agencies, as well as public interest groups, can participate in, and contribute to, an environmental assessment through the AEA process. This integrated systems approach facilitates communication among a diverse group of participants and provides a mechanism for testing potential consequences of various resource actions for all of the interest groups represented. Each participant's perspective of the resource issue is broadened and their understanding of the resource system improved.

Problem Definition and Relevancy of Analysis

Environmental assessments usually are constrained by time and funding. The scope of the impacts to be addressed must be comprehensive in scale, yet prudent in detail. The AEA modeling process results in a workable compromise between breadth and depth and a crisp problem definition. The participation of scientists and policymakers from Federal, State, and local agencies, as well as public interest groups, in the integrated workshop approach helps ensure that data collection and analysis address relevant issues, focus on key questions and variables, and provide information responsive to the needs of decisionmakers.

Interdisciplinary and Interagency Coordination and Research Design

The initial model produced in an AEA workshop may be incomplete. However, the model building and testing process helps identify gaps in available data and in the conceptual understanding of the resource system. Research priorities can be established to fill those data gaps. A clear definition of data requirements for the disciplines and agencies involved in the workshop is explicit in the building of the model. This definition of data requirements can form the basis for interdisciplinary and interagency coordination of data collection and analysis.

Impact Analysis and Evaluation of Analysis Assumptions

Environmental assessments always involve the risk that one or more of the fundamental assumptions on which predictions are based is wrong. The modeling process requires participants to state and evaluate their assumptions about relationships within the resource system. It also provides a mechanism for testing the consequences of basing the model on assumptions that are supported by little or no information. In addition, environmental studies are rarely carried out over a long enough time span to differentiate between natural environmental changes and environmental responses to man-induced stresses. Even preliminary modeling can be a useful tool to simulate different types of development-related changes and the potential consequences of those changes.

Integration and Synthesis of Information

The initial model developed at an AEA workshop provides a framework for integrating existing information about a resource issue and for identifying additional information that is needed. The AEA process is iterative in nature, with time between workshops for research, data collection, and model refinement. Each subsequent workshop integrates information collected since the last workshop, produces a more credible model for the evaluation of management alternatives, and provides for continued communication among agencies and interest grups. The iterative application of the AEA process provides an integrated analysis on which sound resource management recommendations can be based.

BOUNDING AND DEFINING THE RESOURCE OF INTEREST

Any simulation modeling exercise begins with an attempt to bound the system being modeled. Decisions are made about the components that need to be represented in the model and the spatial and temporal scales relevant to those components, even though such decisions may be largely arbitrary for natural systems. The modeling process in the Acid Precipitation Workshops approached the bounding problem through a group discussion of actions and indicators. Actions included those activities that management should consider in their attempt to manipulate the system toward some desired objective. Indicators represented performance measures used to evaluate the response of the system to the various management options. Resolution of spatial and temporal scales is needed so that the model represents the selected components and processes implied by the identified actions and indicators. Spatial resolution constrains the geographic area covered by the model, as well as the degree to which that geographic area needs to be subdivided in order to capture the dynamics of the resource processes involved. Temporal resolution refers to the time-step represented in the model calculations and the number of model iterations needed to cover the time span of interest.

Actions and Indicators

The actions and indicators selected by participants at the Acid Precipitation Workshops are listed in Tables 1 and 2. The actions and indicators were organized into groupings related to the major components (submodels) of the workshop simulation model and edited and combined in order to avoid overlap.

The focus of the Acid Precipitation Workshops was on the identification of priority research needed to improve the assessment of management options related to acid precipitation problems. The various hypotheses concerning system function and mechanisms by which acid precipitation impacts the components of the ecosystem were therefore of greater interest than was the determination of system responses to management strategies. Thus, the list of actions is somewhat shorter than would generally result from a workshop

Table 1. Management actions identified at the Acid Precipitation Workshops.

Model component	Action
Watershed	- Regulate chemical composition of incoming precipitation - Alter canopy cover and composition (evergreen, deciduous, bare ground)
Water Chemistry	- Alter pH of lake or stream
Fish	- Manipulate harvest - Stock species already present - Introduce acid-tolerant species - Introduce metal-tolerant species[a]

[a]Indicates an action identified but not included in the model due to lack of time or information.

Table 2. Indicators (performance measures) identified at the Acid Precipitation Workshops.

Model component	Indicator
Watershed	- Chemical composition of water leaving watershed
Water Chemistry	- Chemical composition of lake and stream
Plankton-Benthos	- Productivity and standing crop - Decomposition rate[a] - Water transparency[a]
Fish	- Species composition - Age and size structure of populations - Harvest or numbers available for harvest - Reproductive success - Heavy metal concentrations[a] - Physical deformities[a] - Behavioral pathologies[a]
Other	- Avian populations[a] - Herpetological populations[a] - Ratio of bacteria to fungi in substrate[a]

[a]Indicates a performance measure identified but not included in the model due to lack of time or information.

designed to explore the potential consequences of alternative management strategies. The mechanisms incorporated into the model, the parameters available to simulate different conditions, and research needs associated with the decision processes implicit in Tables 1 and 2 are discussed later in this report.

Space and Time

Based on the identified actions and indicators, the workshop model was defined around a small watershed in a region of potential sensitivity to acidic inputs. A hypothetical watershed in the Adirondacks area of New York was the object of the first workshop, while watersheds in Ontario and Minnesota were evaluated in subsequent workshops. The watershed, by definition, contained a lake or stream reach, an outflow stream, a tributary stream available for fish spawning, a network of additional tributary streamlets, and a drainage area covered by shallow soils, bare bedrock, and mixed evergreen and hardwood forests. The initial characteristics of the watershed that were chosen for quantification are described in Chapter 8. These characteristics can be changed in order to use the model to simulate conditions in other watersheds.

A basic time-step of 1 week was chosen for the workshop model in order to adequately represent short term events, such as plankton growth and the impact of acid flushing during snowmelt and heavy summer or fall storms. Simulation began on October 1 and the time span of interest was set at 10 to 20 years.

MODEL COMPONENTS AND THE LOOKING OUTWARD MATRIX

The second step in the AEA workshop process is to identify the linkages between the components or submodels by developing a Looking Outward Matrix. The submodels are both the row and column headings of the matrix. The question, "What information is needed from the submodel in this row in order to represent the dynamics of the submodel in this column?" is asked for every block in the matrix that represents the interaction between two components. The actions and indicators that relate to a particular submodel, as well as

the important state variables to be incorporated in that submodel, are listed in the appropriate diagonal matrix blocks. The construction of the matrix identifies linkages between submodel components and is extremely useful in promoting interdisciplinary communication and understanding between workshop participants. Participants must look carefully at the kinds of information they can reasonably expect from other disciplines (i.e., how their submodel dynamics are influenced by other submodels) and the kinds of information other disciplines expect from them (i.e., how their submodel influences the dynamics of other submodels).

The matrix constructed at the Acid Precipitation Workshops was edited to avoid duplication and to eliminate linkages that were originally identified but never incorporated into the model (Fig. 1). For example, the Fish Submodel originally requested data on mercury (Hg) and copper (Cu) concentrations in the lake and stream from the Water Chemistry Submodel. However, insufficient information was available to determine the impact of Hg or Cu concentrations on fish growth or survival and Hg and Cu concentrations were dropped as a linkage, even though they may be important. Identification of data originally requested, but subsequently omitted from the model because of lack of available information, is an important step in identifying data gaps, setting research priorities, and determining needs for model refinement. These information needs are discussed in Chapter 10.

Following the Looking Outward exercise, the workshop participants divided into subgroups in order to construct conceptual submodels representing the internal dynamics of each component. The goals of each subgroup were to describe the mechanisms and processes ("rules for change") that occur in the submodel and to produce a set of indicators of interest and outputs required by other subgroups, given a set of actions that must be represented in the model and a set of inputs from other submodels (Fig. 2). The overall structure of the model resulted from these subgroup interactions and is summarized more fully in the following sections of this report.

FROM THIS SUBMODEL:	THIS SUBMODEL NEEDS INFORMATION CONCERNING: Watershed	Aquatic Chemistry	Plankton/Benthos	Fish
Watershed		Inflows to lake and stream, Concentrations of alkalinity, H, inorganic Al, total Al, Ca, Mg, Na, K, NO_3, SO_4, PO_4, dissolved organic C, and Cl in inflows		
Aquatic Chemistry			Temperature of lake Concentrations of NO_3 (Filson Creek), Phosphorous loadings (Harp Lake)	pH of lake and stream Concentrations of inorganic Al and Ca in lake and stream
Plankton/Benthos		NO_3 uptake (Harp Lake)		Available standing crop of benthos (by size class) in lake and stream Available standing crop of plankton (by size class) in lake
Fish			Food consumed	

Figure 1. Looking Outward Matrix constructed at the Acid Precipitation Workshops.

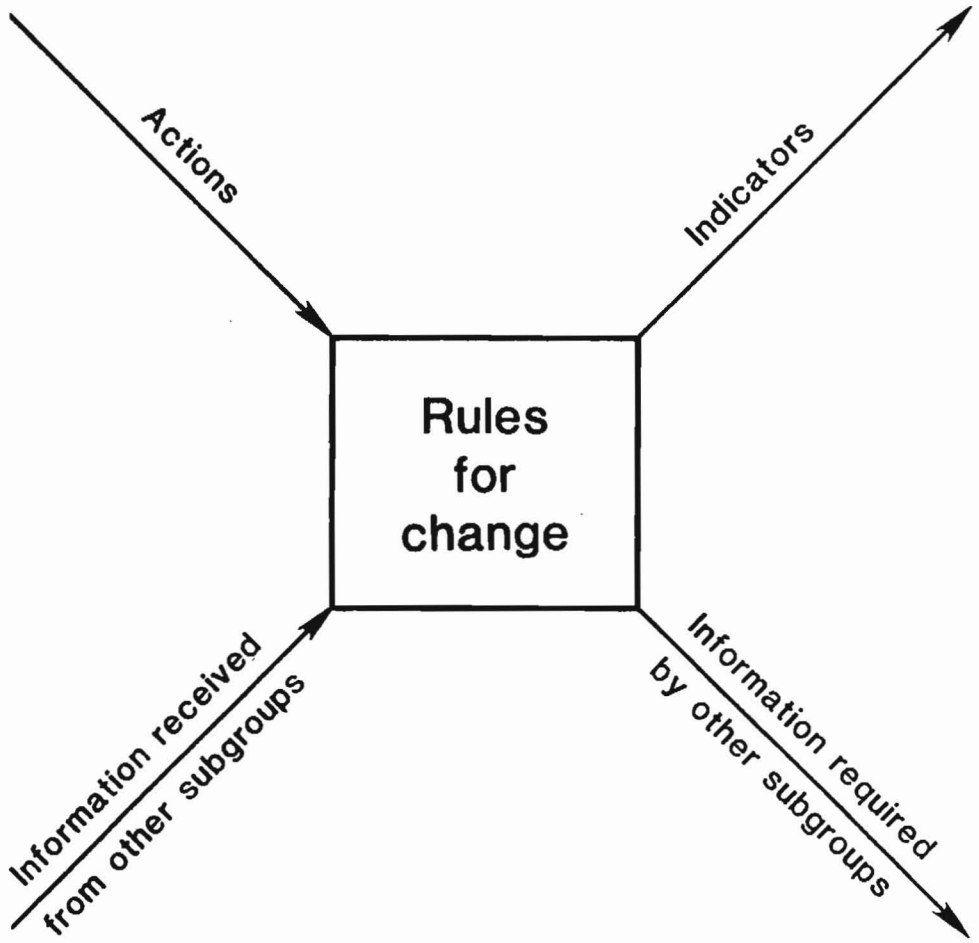


Figure 2. Flow of information to and from each submodel.

3. MODEL STRUCTURE

The preliminary acid precipitation simulation model described here provides a dynamic framework for describing and quantifying the complex interactions between the chemical inputs and outputs from watersheds and the associated chemistry and biota of an aquatic ecosystem. Model inputs which drive the system are referred to as forcing functions. Classical forcing functions in lake ecosystem models include temperature and light regimes and growth-limiting nutrients, such as phosphorous. Stream models often utilize allochthonous organic input as the primary driving force. Acid and other atmospheric inputs and chemicals mobilized by increased acidity create a wide range of additional forcing functions for this model, each of which must be quantified on a seasonal basis. Some degree of knowledge about the baseline condition of each state variable also is required in order to begin the simulation of a specific lake system. Although the present model is not refined enough to provide accurate predictions, the process of building the model provided a mechanism to consider the entire spectrum of important information needed to assess the effects of acid precipitation on aquatic resources.

The descriptive framework supplied by the simulation model integrates state-of-the-art knowledge and is flexible enough to become more sophisticated as additional information is available. The model is composed of four interactive submodels: (1) Watershed; (2) Water Chemistry (stream, lake); (3) Plankton-Benthos; and (4) Fish. Dividing the model into these four component submodels helps organize the consideration and discussion of cause and effect processes reported in the literature. Each submodel is programmed in FORTRAN. The simulation language SIMCON (Hilborn 1973) controls the sequence of model computations, facilitates data input and output, and provides library functions for specialized simulation requirements. Each submodel, except for Water Chemistry, is expressed as a series of difference equations. The Water Chemistry Submodel utilizes a set of chemical equilibrium equations.

Watershed Submodel characteristics are instrumental in determining how susceptible a stream and lake are to the possible adverse effects of anthropogenic or natural inputs of acidity. The Watershed Submodel includes information on precipitation and dry deposition of important chemical constituents and how these inputs are transformed as a function of terrestrial features. Information on atmosphere and watershed chemical inputs to the stream and lake are provided to the Water Chemistry Submodel.

The Water Chemistry Submodel defines the chemical and pH responses of the stream and lake, including the potential compensation and toxic responses of biological communities, to chemical inputs from the atmosphere and the watershed. All major ionic constituents of the aquatic systems are simulated. Chemical characteristics of the stream and lake, calculated by the Water Chemistry Submodel, influence the Plankton-Benthos and Fish Submodels, both metabolically and toxicologically.

The state variables of the Plankton-Benthos Submodel describe the major facets of the lower trophic levels of food chains in streams and lakes. The biological compartments are phytoplankton, zooplankton, and benthos. Zooplankton and benthos are each separated into two size classes to allow for size-selective feeding pressures in the Fish Submodel. Two versions of this submodel can be used, depending on the type of aquatic system being modeled. One version represents lower trophic levels in a stream system driven primarily by allochthonous organic input; the other version represents lower trophic levels in lake systems, driven largely by primary production. Available and unavailable phosphorus are also simulated in the lake version of this submodel, based on the assumption that phosphorus is growth-limiting to phytoplankton.

The Fish Submodel requires information by life stage on a variety of parameters related to growth, survival, reproduction, and the effects of pH and aluminum (Al). The submodel also requires estimates of annual harvest for areas where angling pressure is significant. Fisheries dynamics, in terms of the number of individuals, average weight, and average length by life stage for brook trout and white sucker populations, are described by the Fish Submodel. The submodel can also be used to compare spawning activities in the lake (or stream reach) with spawning activities in the inflow streams, which

are affected by acid precipitation to a much greater extent than the lake. The state variables in the Fish Submodel define a minimum data set from which changes in fish biomass and production can be computed. Changes in these variables are related to the supply of invertebrate food items (information on available food is obtained from the Plankton-Benthos Submodel) and the toxic effects of pH and Al concentration on reproduction and mortality. Data on pH and inorganic Al concentrations are obtained from the Water Chemistry Submodel.

The Acid Precipitation Workshops resulted in a cooperatively developed modeling framework that can be used to simulate the important variables in a variety of aquatic systems. This model represents selected known interactions, rather than an attempt to recreate the real world, and will increse in sophistication and credibility as more information becomes available. The development of this model resulted in the identification of data gaps that need to be filled before a more accurate description of lake and biotic responses to acid precipitation can be made.

A model, such as the one developed during the Acid Precipitation Workshops, might eventually link atmospheric transfer, chemical transformation, and deposition models for sulfate and nitrate ions. The resulting model would more completely address the acid precipitation problem, starting with the production of oxides of sulfur and nitrogen and ending with the effects of the oxides on natural resources.

4. WATERSHED SUBMODEL

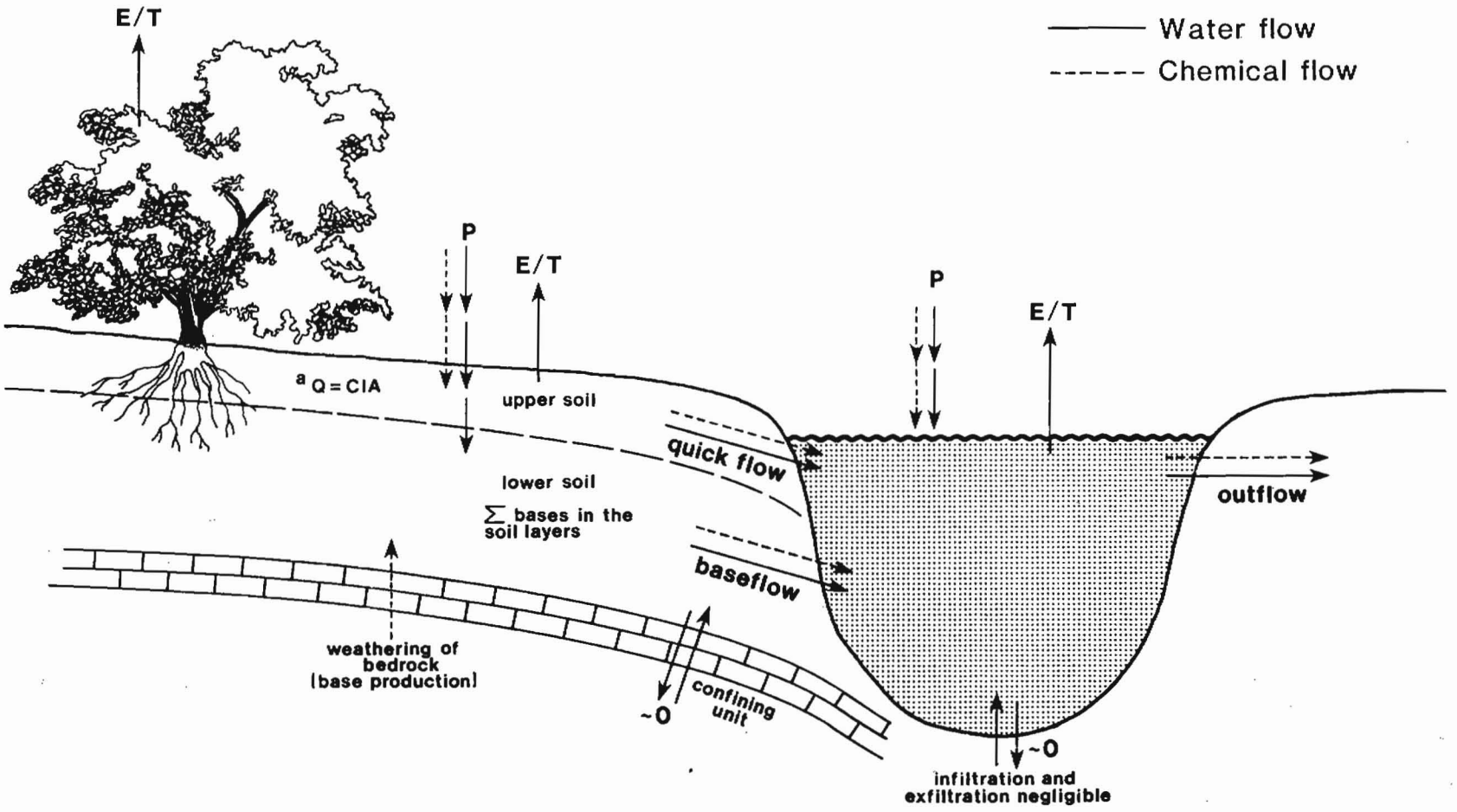
SCOPE

The Watershed Submodel is designed to: (1) compute the system hydrology or, in effect, route water from precipitation to stream discharge; (2) compute water chemistry parameters entering the stream system (Ca^{+2}, Mg^{+2}, Na^{+}, K^{+}, SO_4^{-2}, NO_3^{-}, Cl^{-}); and (3) provide a continuous computation of the bases in the soil.

MODEL APPROACH

The Watershed Submodel is not intended to be geochemically specific in its treatment of solute acquisition in the watershed. An empirical approach was chosen because this form was expected to be readily applicable to a wider variety of circumstances and because of the complexity of weathering reactions. Some chemical and physical factors, such as the spatial distribution of minerals within the watershed, mineral dissolution kinetics, mineral/water contact time, the role of organics in modifying mineral dissolution rates, and overland versus soil seepage flow, are not directly represented. Results of efforts such as the EPRI Integrated Lake-Watershed Acidification Study (Electric Power Research Institute 1981) should be useful if this submodel is upgraded in the future. The present procedure uses monitoring data from calibrated watersheds to determine correlations between stream flows and chemical concentrations. This approach should provide a broad spectrum of conditions with which to test biological responses to acidification. The applicability of the model will be even greater once data sets from watersheds with a wide variety of geochemical and morphological regimes are included.

A conceptual diagram of the Watershed Submodel is presented in Figure 3. Water is input to the ecosystem via precipitation and then enters the soil



[a] 100% runoff (c - 1.0) is assumed during snowmelt periods

Figure 3. Watershed hydrologic and base cation chemical balance.

environment. A portion of the water entering the system is lost by evapotranspiration. Movement of remaining water is tracked through an upper (O and A horizons) and a lower (B and C horizons) soil layer. Water associated with the upper soil layer is termed quickflow, while water associated with the lower soil environment is termed baseflow. Water quality parameters are computed by an empirical concentration-discharge relationship. Soil chemistry is monitored by computing the basic cation (Ca^{+2}, Mg^{+2}, Na^{+}, and K^{+}) content of the soil system. This computation is made by performing a mass balance on cations in the soil system, which includes cations entering via precipitation and soil weathering, as well as cations exported from the soil through waterflow and vegetative uptake.

COMPUTATIONAL APPROACH AND PARAMETER ESTIMATES

The calculation sequence for the Watershed Submodel is summarized in Figure 4. Input and state variables are listed in Figure 5.

Hydrology Calculations

The hydrology calculations use weekly values for rain and snow, modified by a small random component, as input data. The simulation year is divided into two portions, one when precipitation falls as rain, the other when precipitation falls as snow. In the absence of an ice covering, rain and snow falling on the lake surface are simply added to the volume of the lake. Precipitation occurring when an ice cover is present (specified by setting values for the weeks of ice formation and ice melt) is accumulated and added to the volume of the lake during the week that the ice melts.

Hydrology calculations pertaining to the land portion of the watershed are done on a unit-area basis (1 m^2) and accumulated for the entire watershed at the end of the calculation sequence. Precipitation for each m^2 of surface area in the watershed is first reduced by a weekly evapotranspiration factor. Any snow remaining after evapotranspiration losses is added to the snow remaining at the end of the previous week. Prior to the spring snowmelt period (assumed to begin in the week that precipitation stops falling as snow), snow

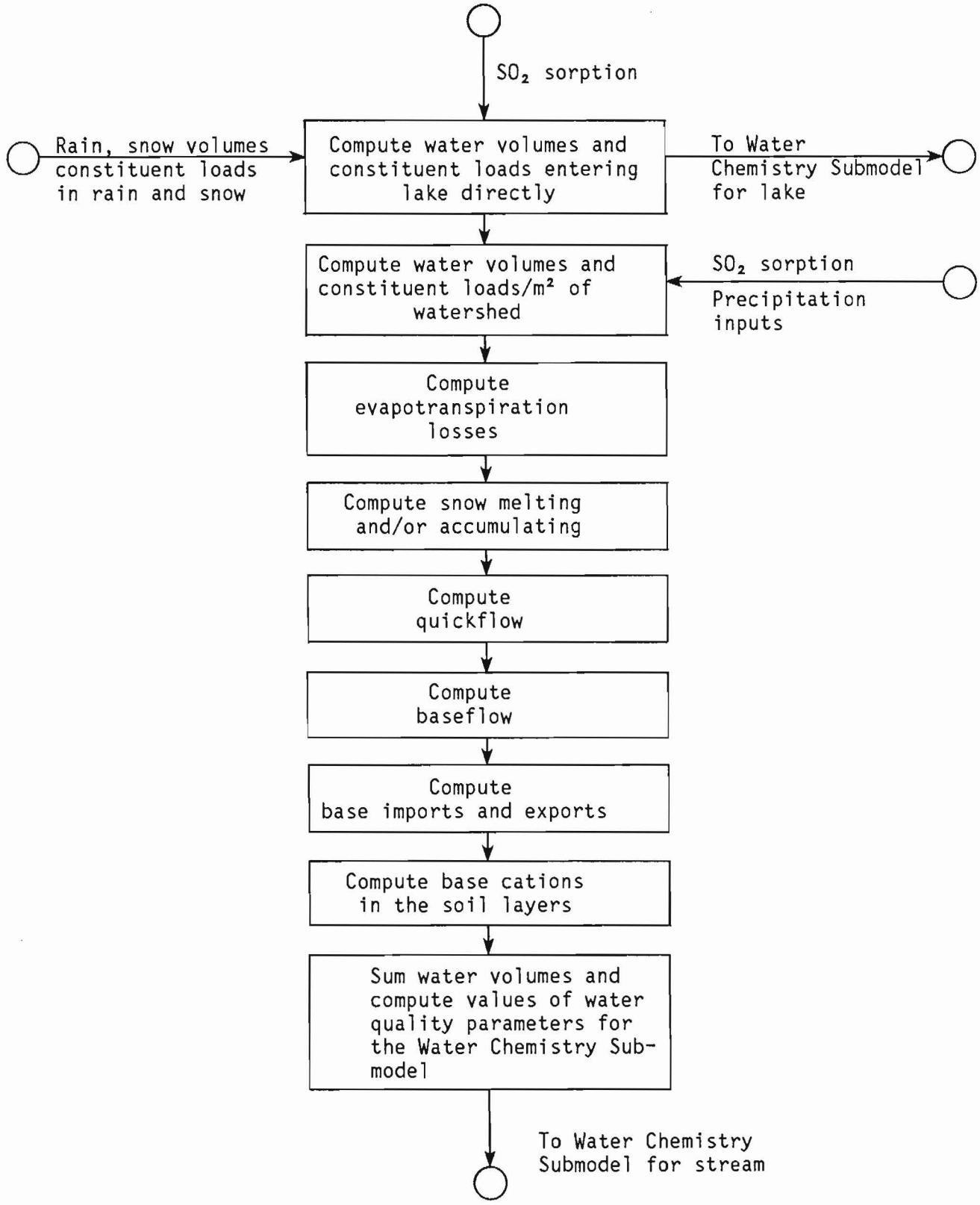


Figure 4. Calculation sequence in the Watershed Submodel.

Input Variables

Weekly precipitation volume

Weekly atmospheric loadings of Ca^{+2}, Mg^{+2}, Na^{+}, K^{+}, NO_3^{-}, SO_4^{-2}, and Cl^{-}

Soil depth in two layers

Exchangeable basic cation denisty in two soil layers

Average porosity of two soil layers

Bulk density of two soil layers

Depositional velocity of SO_2

Gaseous SO_2 concentration

Weekly evapotranspiration

Concentration-discharge coefficients

Vegetation nitrogen and sulfur uptake coefficients

Periods of biological activity/inactivity

Periods of rain/snow precipitation

Period when ice cover is present on lake

Vegetation uptake of basic cations

Weathering release of basic cations

State Variables

Watershed discharge from two soil layers

Concentrations of Ca^{+2}, Mg^{+2}, Na^{+}, K^{+}, NO_3^{-}, SO_4^{-2}, and Cl^{-} input to the stream

Sum of basic cations in two soil layers

Figure 5. Variables for the Watershed Submodel.

is calculated as melting at a user-specified maximum rate. Snow in excess of this maximum rate is accumulated as snowpack. During the period of spring snowmelt, a constant percentage of the accumulated snowpack is calculated as melting each week.

Water resulting from snowmelt and from precipitation falling as rain is routed through the two soil layers as either quickflow (surface flow plus interflow through the upper soil layer) or baseflow (flow through the lower soil layer). All snowmelt is assumed to move as quickflow. Additional quickflow resulting from precipitation in the form of rain is computed from the rational equation (Gray 1970):

$$Q = c * I * A \tag{1}$$

where Q = rate of runoff (l/week)
c = runoff coefficient
I = rainfall intensity (l/m^2/week)
A = area of the watershed (m^2)

While the rational method is intended for use in determining peak flow for small watersheds for a single precipitation event, it generates discharge patterns that are similar to observed data and suitable for use in the remainder of the model.

Water remaining after the quickflow calculation is assumed to percolate through to the lower soil layer and is added to any soil moisture remaining from the previous week. If this quantity of water is greater than the storage capacity of the lower layer (determined from soil depth and porosity information), the excess is added to the quickflow. Baseflow through the lower soil layer is calculated according to the formula:

$$y = a * e^{-b(c-x)} \tag{2}$$

where y = baseflow (l/m^2)
a = maximum baseflow rate (occurring at soil saturation) (l/m^2)
b = a constant governing the shape of the curve
c = maximum soil moisture storage (soil depth x porosity) (l/m^2)
x = current soil moisture storage (l/m^2)

The function is constrained in the model so that baseflow can never be greater than the current amount of stored soil moisture.

Water Chemistry Calculations

Water chemistry parameters (Ca^{+2}, Mg^{+2}, Na^{+}, K^{+}, SO_4^{-2}, NO_3^{-}, and Cl^{-}) are simulated using an empirical concentration-discharge model (Johnson et al. 1969), even though such an approach is not entirely satisfactory from a mechanistic standpoint. Several potential problems with using a mechanistic model prompted this choice. For example, the watershed is an extremely complicated environment. Vegetative nutrient cycling, weathering reactions, soil chemistry, soil microbial transformations, and other reactions are extremely difficult to model. Little is known of the kinetics of mineral dissolution and microbial transformations, soil exchange adsorption equilibria, gaseous exchange reactions, and many other components of the watershed environment. In addition, kinetic and equilibrium constants and soil, mineral, and vegetation characterization information would not be readily available for most systems if a complex mechanistic model was formulated.

Precipitation constituents for a given week are input to the model and enter the watershed or the lake by direct impact. Those constituents that enter the lake directly represent an input to the Water Chemistry Submodel (Fig. 8, Chapter 5). Only two constituents deposited in precipitation (sulfate and nitrate) directly influence stream chemistry values. Concentrations of other constituents are computed from stream discharge. This is, in essence, assuming that watershed cycling of nutrients (other than sulfur and nitrogen) is not influenced by changes in atmospheric loading.

The concentration discharge model utilized by Johnson et al. (1969) is baed on the concept of stream chemistry as a blending of two waters, quickflow and baseflow, with distinct water chemistry. Baseflow is water of relatively high ionic strength. Stream water quality composition approaches that of baseflow as discharge approaches zero. As discharge increases, baseflow is mixed in the appropriate ratio with quickflow. Quickflow is a relatively dilute water and is somewhat representative of precipitation chemistry. The concentration-discharge relationship is:

$$X = \frac{Z2}{1 + Z1 * D} + Z3 \quad (3)$$

where X = parameter concentration (mg/l)
D = stream discharge (l/ha/day)
Z1, Z2, Z3 = empirical constants

Baseflow concentration can be approximated by summing the empirical constants Z2 and Z3 because stream water quality composition approaches that of baseflow as discharge approaches zero.

Concentrations of nitrate and potassium are strongly influenced by watershed vegetation. Therefore, two concentration-discharge relationships are utilized. One relationships is appropriate for the biologically active period; the other is appropriate for the biologically inactive period. The biologically active and biologically inactive periods are specified for each individual system.

The concentration-discharge relationships are modified for sulfate and nitrate to accommodate changes in gaseous SO_2 and sulfate and nitrate acid loadings above those that occurred when data for determining concentration-discharge relationships were collected. Bulk precipitation data are used in the Watershed Submodel; that is, precipitation includes wetfall and dry deposition due to particulate and aerosol sedimentation. Deposition of SO_2 gas by sorption onto vegetation and soil is included separately. Changes in SO_2 deposition due to changes in SO_2 concentration (from ambient levels existing when concentration-discharge data were obtained) are represented as the product of the change in SO_2 concentration and the depositional velocity:

$$D = V * S * K \quad (4)$$

where D = change in gaseous deposition from ambient levels (mg SO_4/m^2/week)
V = depositional velocity (cm/sec)
S = change in SO_2 concentration from ambient levels (μg SO_2/m^3)
K = dimensional conversion to yield mg SO_4/m^2/week (9.07)

Changes in sulfate and nitrate loading to the ecosystem (H_2SO_4 or HNO_3) from bulk deposition are modified by vegetative uptake. A fraction of the sulfate and nitrate entering the ecosystem is assimilated by the terrestrial system. This uptake produces an equivalent amount of hydroxide, which neutralizes the associated hydrogen ion, assuming electroneutrality. Net changes in sulfate (including gaseous SO_2 concentration changes) and nitrate (the amount entering less vegetative uptake) are added to the concentration-discharge values that were determined. The water quality parameter values are utilized in basic soil cation balance calculations and are input to the Water Chemistry Submodel.

Soil Cation Mass Balance Calculations

In this model, a mass balance is calculated for the basic cations in the two soil layers (Fig. 6). The depth, bulk density, and cation exchange capacity of each soil layer are inputs to the Watershed Submodel (Fig. 5). Cations are lost from the system due to export in streamflow and vegetation uptake. Additions to the system occur through precipitation and weathering of bedrock.

The concentration-discharge relations estimate the total base cations exported from the watershed; it is necessary to separate the total into its quickflow and baseflow components. The baseflow component for each cation is determined experimentally or approximated from equation (3) (Z2 + Z3). The quickflow component is obtained for each cation by solving the mass balance equation for QB:

$$C = \frac{BF * BB + QF * QB}{F} \tag{5}$$

where C = stream concentration (mg/l)
BF = baseflow (l)
BB = concentration in baseflow (mg/l)
QF = quickflow (l)
QB = concentration in quickflow (mg/l)
F = streamflow (l)

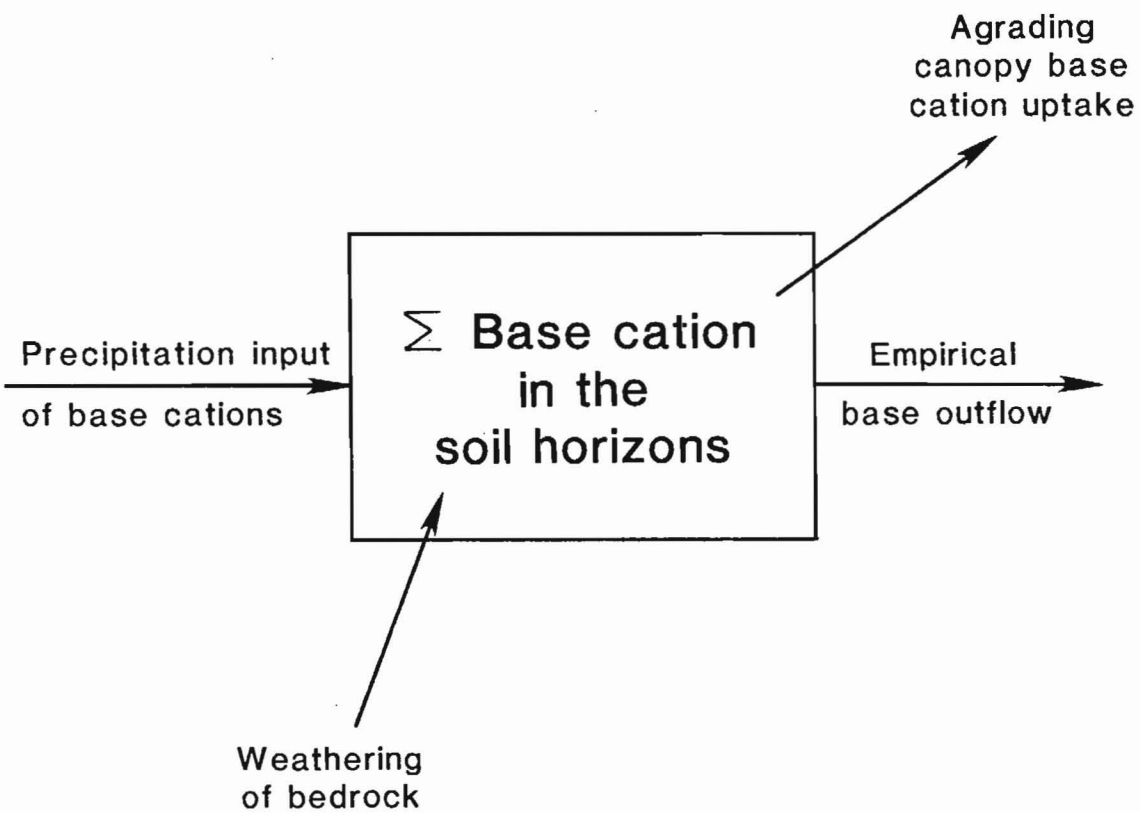


Figure 6. Mass balance on sum of the base cations in the soil horizons.

Individual cation concentrations are converted to mg/l of $CaCO_3$ and summed for later use in calculating changes in the cation reservoirs in the two soil layers.

The mass balance on base cations assumes that:

(1) export of bases is independent of pH and inversely dependent on stream discharge (cf Johnson et al. 1969);

(2) uptake of cations by vegetation releases protons to the system in an aggrading forest system (base uptake); and

(3) weathering of bedrock (siliceous material) results in alkalinity or base-associated cations available to the lower soil layer.

The first assumption is clearly an oversimplification. Export of bases depends on the saturation of bases in the soils and an improvement to the model would be to link base export to the amount of bases remaining in the soil horizons. This relationship could utilize the mass balance on soil bases described below.

The hydrologic budget and the soil base cation balance are based on the principal of continuity of mass. Hydrologically, total flow into the upper soil compartment equals the total flow to the stream plus water which percolates to the lower soil layer. Storage of water in the lower soil profile was discussed earlier. Titration of soil bases is accomplished by a mass balance on base cations. The following equations are solved iteratively at each time step:

$$BUP_t = BUP_{t-1} + BP - QB \qquad (6)$$

where BUP = sum of the bases in the upper soil layer
BP = sum of the bases in precipitation
QB = sum of the bases in the quickflow

$$BLO_t = BLO_{t-1} + BW - BB - BV \tag{7}$$

where BLO = sum of the bases in the lower soil layer
BW = sum of the bases from weathering of bedrock
BB = sum of the bases in the baseflow
BV = sum of the bases taken up by vegetation

All quantities in equations (6) and (7) need to be expressed in eq/m³. Conversion to eq/m³ is accomplished with the following computations. An initial estimate of the sum of the bases in the upper soil layer in eq/m³ is obtained from:

$$BUP = BI * BDUP * K \tag{8}$$

where BUP = initial sum of bases in upper soil layer (eq/m³)
BI = sum of bases in upper soil layer (meq/100 g)
BDUP = bulk density of upper soil layer (g/cm³)
K = dimensional conversion to yield eq/m³ (10)

A corresponding calculation is performed to obtain the sum of the bases in the lower soil layer. In successive iterations, the terms in equation (6) are obtained and summed in units of eq/m³ according to the equation:

$$BUP_t = BUP_{t-1} + \frac{BP}{DUP} - \frac{QB * QF * K}{DUP * WA} \tag{9}$$

where BUP = sum of the bases in the upper soil layer (eq/m³)
BP = sum of the bases in precipitation (eq/m²)
DUP = depth of upper soil layer (m)
QB = sum of the bases in quickflow (mg/l as $CaCO_3$)
QF = quickflow (l)
WA = watershed surface area (m²)
K = dimensional conversion from mg $CaCO_3$ to eq (2×10^{-5})

Similarly, the terms in equation (7) are obtained and summed in units of eq/m³ according to the equation:

$$BLO_t = BLO_{t-1} + \frac{BW}{DLO} - \frac{BB * BF * K}{DLO * WA} - \frac{BV}{DLO} \quad (10)$$

where BLO = sum of the bases in the lower soil layer (eq/m^3)
BW = sum of the bases due to weathering (eq/m^2)
DLO = depth of lower soil layer (m)
BB = sum of the bases in baseflow (mg/l as $CaCO_3$)
BF = baseflow (l)
WA = watershed surface area (m^2)
BV = sum of the bases taken up by vegetation (eq/m^2)
K = dimensional conversion from mg $CaCO_3$ to eq (2×10^{-5})

Chapter Authors: Jerry Schnoor, University of Iowa; Joe Eilers, Wisconsin Department of Natural Resources; Charles Driscoll, Syracuse University; and Wolfgang Scheider, Ontario Ministry of the Environment.

Chapter Contributors (in alphabetical order): Wes Bradford, U.S. Geological Survey; Tom Burton, Michigan State University; Patricia Carstensen, FWS; Robert Friedman, Office of Technology Assessment; A. J. Johannes, Rensselaer Polytechnic Institute; Richard Johnson, FWS; Rick Linthurst, North Carolina State University; and Orie Loucks, Institute of Ecology.

5. WATER CHEMISTRY SUBMODEL

SCOPE

The Water Chemistry Submodel consists of two subsystems, the stream subsystem and the lake subsystem. Water chemistry modeling is done separately for the two subsystems. Hydrologic and associated chemical inputs enter the stream environment from the terrestrial system. Stream water and direct atmospheric inputs enter the lake environment. Lake water and associated chemical constituents are exported via the lake outlet. Chemical characteristics of the stream and lake calculated by the Water Chemistry Submodel influence the Fish and Plankton-Benthos Submodels, both metabolically and toxicologically.

MODEL APPROACH

A number of equilibrium models and associated programs are available for calculating the mobilization of chemical species in natural waters (e.g, Truesdell and Jones 1974; Westall et al. 1976). These models are thermodynamically rigorous, although shortcomings exist regarding metal-ligand complexation constants and geochemically important solid-solution reactions. The thermodynamic approach is vulnerable, however, when metal species and concentrations must be evaluated. This is because elements, such as Cu, Zn, Cd, Pb, and Hg, are greatly influenced by interactions with suspended biotic and abiotic components in the water column.

The overall model is designed to focus on biological effects of changes in water quality parameters, rather than respond to the geochemical rigor discussed above. The Water Chemistry Submodel could, ultimately, incorporate more sophisticated subroutines on solution chemistry if they are needed. The present approach to calculating the titration reactions from stream and lake parameters and the hydrogen ion input from precipitation is expected to be adequate for simulating a wide range of realistic biological responses.

The chemical composition of the stream and lake systems is computed in the Water Chemistry Submodel (Fig. 7), based on ionic electroneutrality. All major ionic constituents are monitored (Fig. 8). Water quality parameters (Ca^{+2}, Mg^{+2}, Na^{+}, K^{+}, SO_4^{-2}, NO_3^{-}, and Cl^{-}) enter the aquatic environment from the Watershed Submodel. Water quality parameters (dissolved organic carbon (DOC), ammonium (NH_4), total fluoride (F_t), phosphorus (P), and temperature), of which little is known with respect to metabolism in the terrestrial environment, are directly entered in the stream. Known concentrations from representative streams are utilized for these inputs. The remaining parameters of interest, inorganic carbon and aluminum, are calculated from thermodynamic equilibrium relationships with atmospheric CO_2 and solid phase aluminum ($Al(OH)_3$), respectively.

Calculations are made for the stream system from inputs from the terrestrial environment of the Watershed Submodel. Calculated stream constituents are then exported to the lake. Lake chemistry is also influenced directly by precipitation and algal metabolism of nutrients. Net algal uptake of nitrate results in a release of base equivalents to the aquatic environment. This increases lake alkalinity and pH. Lake and stream component composition are both computed by an electroneutrality balance. Lake pH, aluminum, and alkalinity values are calculated when system electroneutrality is established. This represents the solution composition exported from the lake through the lake outlet.

Water chemistry of lake and stream environments may be modified by the addition of chemicals during aquatic restoration efforts. These may include an addition of bases (e.g., lime) for the stream and bases or nutrients (phosphorus) for the lake.

COMPUTATIONAL APPROACH AND PARAMETER ESTIMATES

The computational strategy for the Water Chemistry Submodel is summarized in Figure 9. Constituent values that are input are initially calculated in moles per liter. Aqueous pH and free fluoride values must be estimated in order to evaluate thermodynamic relationships for inorganic carbon, dissolved organic carbon, aluminum, and fluoride.

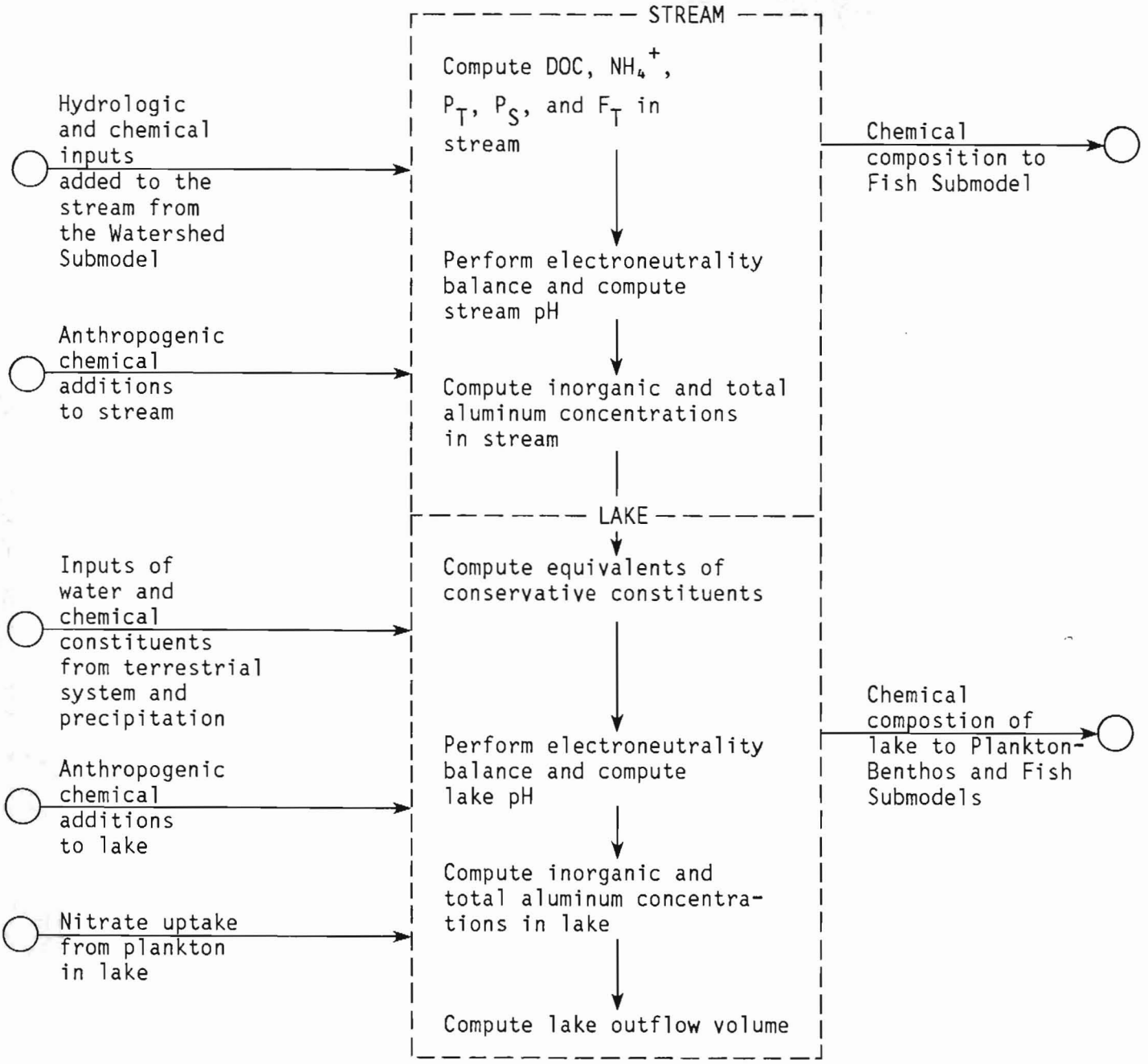


Figure 7. Calculation sequence for the Water Chemistry Submodel.

Input Variables

Stream inputs

Ca^{+2}, Mg^{+2}, Na^{+}, K^{+}, SO_4^{-2}, NO_3^{-}, Cl^{-}, P, discharge volume

Precipitation inputs

Ca^{+2}, Mg^{+2}, Na^{+}, K^{+}, SO_4^{-2}, NO_3^{-}, Cl^{-}, P, H^{+}, precipitation volume

Direct inputs

DOC, P, NH_4^{+}, total fluoride

Plankton inputs

NO_3^{-} uptake

Thermodynamic inputs

P_{CO_2}, K_{SO} for $Al(OH)_3$

Management strategy inputs

addition of bases (e.g., lime), nutrients

State Variables

Stream state variables

pH, alkalinity, total aluminum, inorganic aluminum

Lake state variables

Ca^{+2}, Mg^{+2}, Na^{+}, K^{+}, SO_4^{-2}, NO_3^{-}, Cl^{-}, P, DOC, NH_4^{+}, pH, alkalinity, total aluminum, inorganic aluminum

Output Variables

Stream output variables

pH, alkalinity, total aluminum, inorganic aluminum

Lake output variables

Ca^{+2}, Mg^{+2}, Na^{+}, K^{+}, SO_4^{-2}, NO_3^{-}, Cl^{-}, P, DOC, NH_4^{+}, pH, alkalinity, total aluminum, inorganic aluminum, total evaporation, lake temperature, lake outflow

Figure 8. Variables for the Water Chemistry Submodel.

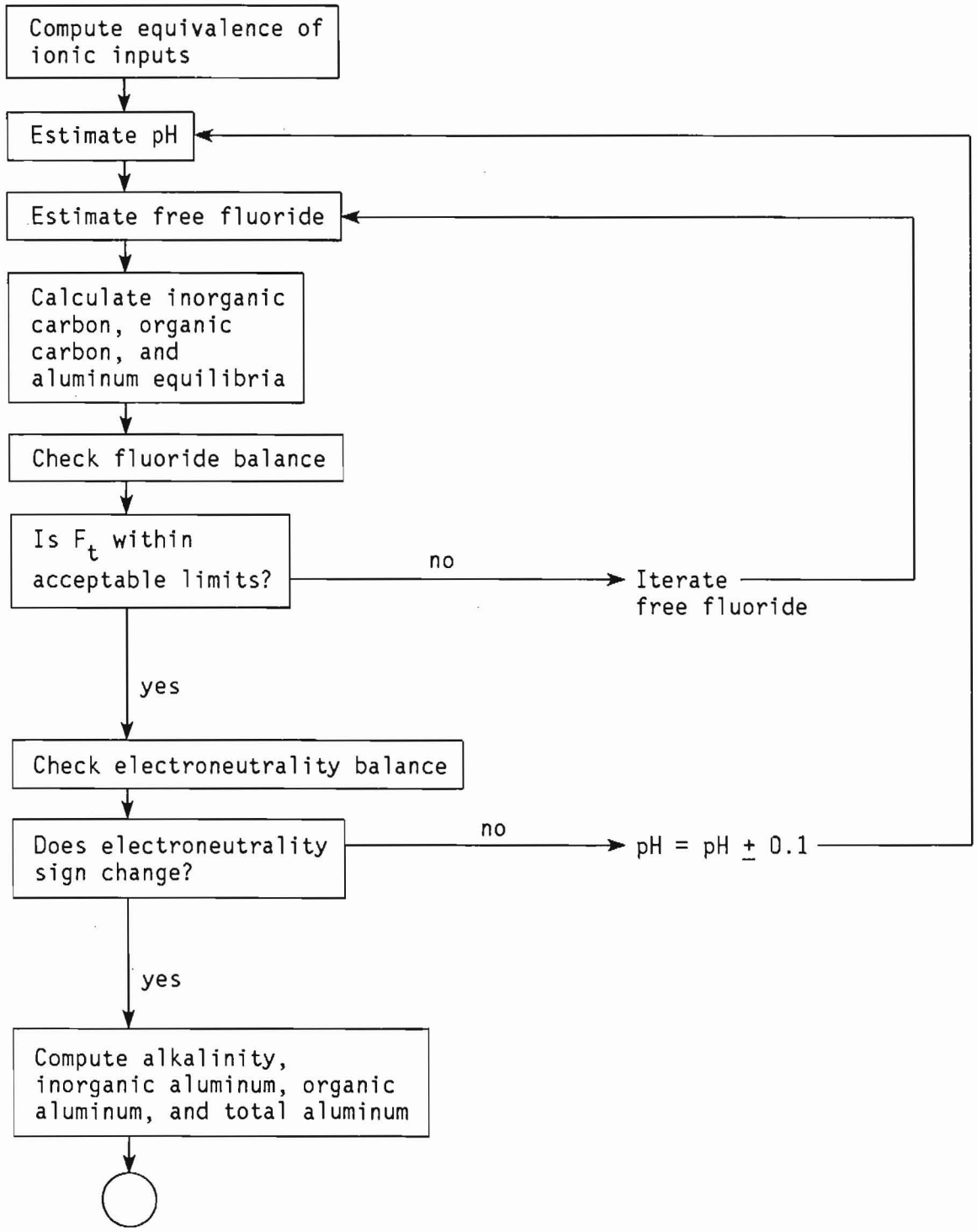


Figure 9. Computation of solution electroneutrality.

The system is assumed to be in equilibrium with atmospheric CO_2 for the inorganic carbon calculations. Therefore, the input variable partial pressure of atmospheric CO_2 (P_{CO}) is utilized (Stumm and Morgan 1970):

$$[HCO_3^-] = \frac{10^{-6.3} * 10^{-1.5} * P_{CO_2}}{[H^+]} \tag{11}$$

$$[CO_3^{-2}] = \frac{[HCO_3^-] * 10^{-10.3}}{[H^+]} \tag{12}$$

Two relationships are utilized in order to evaluate dissolved organic carbon acid/base chemistry. The first is an empirical relationship between dissolved organic carbon and dissolved organic carbon acid/base equivalents (Ct) (Driscoll 1980):

$$Ct = (2.62 * 10^{-6}) * DOC + (7.63 * 10^{-6}) \tag{13}$$

The other relationship involves an organic carbon proton dissociation constant (pKa = 4.41). These values are utilized to compute the pH-dependent organic carbon base equivalents ($RCOO^-$) (Driscoll 1980):

$$[RCOO^-] = \frac{(Ct * 10^{-4.41})}{([H^+] + 10^{-4.41})} \tag{14}$$

The various dissolved aluminum species are assumed to be in equilibrium with an $Al(OH)_3$ mineral phase. The following equilibrium calculations (Burrows 1977), utilizing the solubility constant (K_{so}), are made for this mineral phase:

$$[Al^{+3}] = [H^+]^3 * Kso \tag{15}$$

$$[Al(OH)^{+2}] = \frac{[Al^{+3}] * 10^{-4.99}}{[H^+]} \tag{16}$$

$$[Al(OH)_2^+] = \frac{[Al^{+3}] * 10^{-10.13}}{[H^+]^2} \tag{17}$$

$$[Al(OH)_4^-] = \frac{[Al^{+3}] * 10^{-22.2}}{[H^+]^4} \tag{18}$$

$$[AlF^{+2}] = [Al^{+3}] * [F^-] * 10^{7.02} \tag{19}$$

$$[AlF_2^+] = [Al^{+3}] * [F^-]^2 * 10^{12.76} \tag{20}$$

$$[AlSO_4^+] = [Al^{+3}] * [SO_4] * 10^{3.21} \tag{21}$$

The total fluoride is calculated, based on the above values, for aluminum fluoride complexes:

$$F_T = [F\ ] + [AlF] + [AlF_2] \tag{22}$$

The calculated F_T is compared with the input total fluoride value. If it is within acceptable limits, the model proceeds; otherwise, the free fluoride estimate is increased or decreased according to the relative magnitude of F_T to the input fluoride value and the cycle rerun.

An electroneutrality calculation is performed after all thermodynamic calculations are made:

$$\begin{aligned} EN = {} & 2[Ca^{+2}] + 2[Mg^{+2}] + [Na^+] + [K^+] + 3[Al^{+3}] \\ & + 2[Al(OH)^{+2}] + [Al(OH)_2^+] + 2[AlF^{+2}] + [AlF_2^+] \\ & + [AlSO_4^+] + [NH_4^+] - [Al(OH)_4^-] - 2[SO_4^{-2}] - [NO_3^-] \\ & - [Cl^-] - [HCO_3^-] - 2[CO_3^{-2}] - [RCOO^-] - [OH^-] + [H^+] \end{aligned} \tag{23}$$

The electroneutrality balance (EN) is checked. A positive value for EN signifies a cation excess, in which case the pH is incremented to a higher value. The pH is decremented to a lower value if EN is negative. The iteration proceeds until a sign change of the electroneutrality balance (EN) occurs, indicating that the system is in ionic balance.

Alkalinity, organic aluminum (Al-organic), inorganic aluminum (Al-inorganic), and total aluminum (Al-total) are computed when the iterative routine is completed:

$$\text{Alkalinity} = [HCO_3^-] + 2[CO_3^{-2}] + [RCOO^-] \tag{24}$$

$$+ [Al(OH)^{+2}] + 2[Al(OH)_2^+] + 4[Al(OH)_4^-] + [OH^-] - [H^+]$$

$$[\text{Al-organic}] = [1.7 * 10^{-6} * DOC] - 3.26 * 10^{-6} \tag{25}$$

$$[\text{Al-inorganic}] = [Al^{+3}] + [Al(OH)^{+2}] + [Al(OH)_2^+] + [Al(OH)_4^-] \tag{26}$$

$$+ [AlF^{+2}] + [AlF_2^+] + [AlSO_4^+]$$

$$[\text{Al-total}] = [\text{Al-inorganic}] + [\text{Al-organic}] \tag{27}$$

The organic aluminum equation is an empirical relationship. This technique is utilized to compute the ionic equilibrium for both stream and lake chemistry. Thermodynamic computations do not include temperature or ionic strength corrections, although these corrections might improve the model.

Chapter Author: Charles Driscoll, Syracuse University.

Chapter Contributors: (in alphabetical order) Jay Bassin, FWS; Ron Eisler, FWS; Dale Hoffman, FWS; Arnold Julin, FWS; Gordon Omen, University of Montana; and Monta Zengerle, EPRI.

6. PLANKTON-BENTHOS SUBMODEL

SCOPE

The Fish Submodel requires information about the food source for fish, which is provided by the Plankton-Benthos Submodel. Several approaches to developing food source information were explored. A relatively detailed formulation of the chemical, physical, and biological processes controlling algal productivity and food chain components providing trophic support of fish populations was developed for a lacustrine system and parameterized to the extent possible for Harp Lake, Ontario. A less detailed, empirical formulation, based on the morphoedaphic index (Ryder et al. 1974), was also proposed and explored as an alternative to provide a general bound on the trophic status of a lake. This information is described in the following section on the Harp Lake model approach, but is not utilized elsewhere.

A model with a different structure seemed appropriate to represent trophic support of fish in a stream such as Filson Creek. The approach taken was to adapt the relevant aspects of an existing stream model (Colby and McIntire 1978; McIntire and Colby 1978).

MODEL APPROACH

Harp Lake

Detailed formulation. Seven state variables, five biological and two chemical, are simulated in the lacustrine Plankton-Benthos Submodel. The biological state variables are phytoplankton biomass, two zooplankton biomass compartments based on size (< 1 mm and ≥ 1 mm), and two benthos compartments, also based on size. Phytoplankton dynamics are assumed to be phosphorus limited in this submodel, because of the generally oligotrophic nature of lakes known to be susceptible to acid precipitation. Phosphorus components are simulated and their loadings input to the submodel. The chemical state

variables are operationally defined as a biologically unavailable and a biologically available phosphorus pool. Information on net nitrate consumption is also provided to the Water Chemistry Submodel for use in the claculation of total alkalinity.

The basic calculation sequence for the lacustrine Plankton-Benthos Submodel is shown schematically in Figure 10. The difference equations which describe the model formulation are presented in Equations 28-34:

Δ unavailable phosphorus/Δ time = import + phytoplankton release + zooplankton release - mineralization - sinking - export (28)

Δ available phosphorus/Δ time = import - phytoplankton uptake + mineralization - export (29)

Δ phytoplankton biomass/Δ time = growth - sinking - zooplankton grazing - export - other mortality and respiration (30)

Δ small zooplankton biomass/Δ time = assimilation of phytoplankton - respiration - fish predation - other mortality - export (31)

Δ large zooplankton biomass/Δ time = assimilation of phytoplankton - respiration - fish predation - other mortality - export (32)

Δ small benthos biomass/Δ time = net growth - fish predation - other mortality (33)

Δ large benthos biomass/Δ time = net growth - fish predation - other mortality (34)

All rates used in these equations are in units of day^{-1}. Each equation is applied over a shorter time step (0.1 day); submodel output is weekly.

Empirical formulation. The detailed lacustrine Plankton-Benthos Submodel has rather complex data requirements, which limit its usefulness over a wide range of sites. A simpler alternative was sought as an optional substitute. The assumption underlying the simpler approach is that the direct effects of Al and pH on fish in terms of toxicity and reduced growth are more important than the secondary impact of altered food supply. Some relationship is still required, however, to express the capacity of a lake to support fish growth.

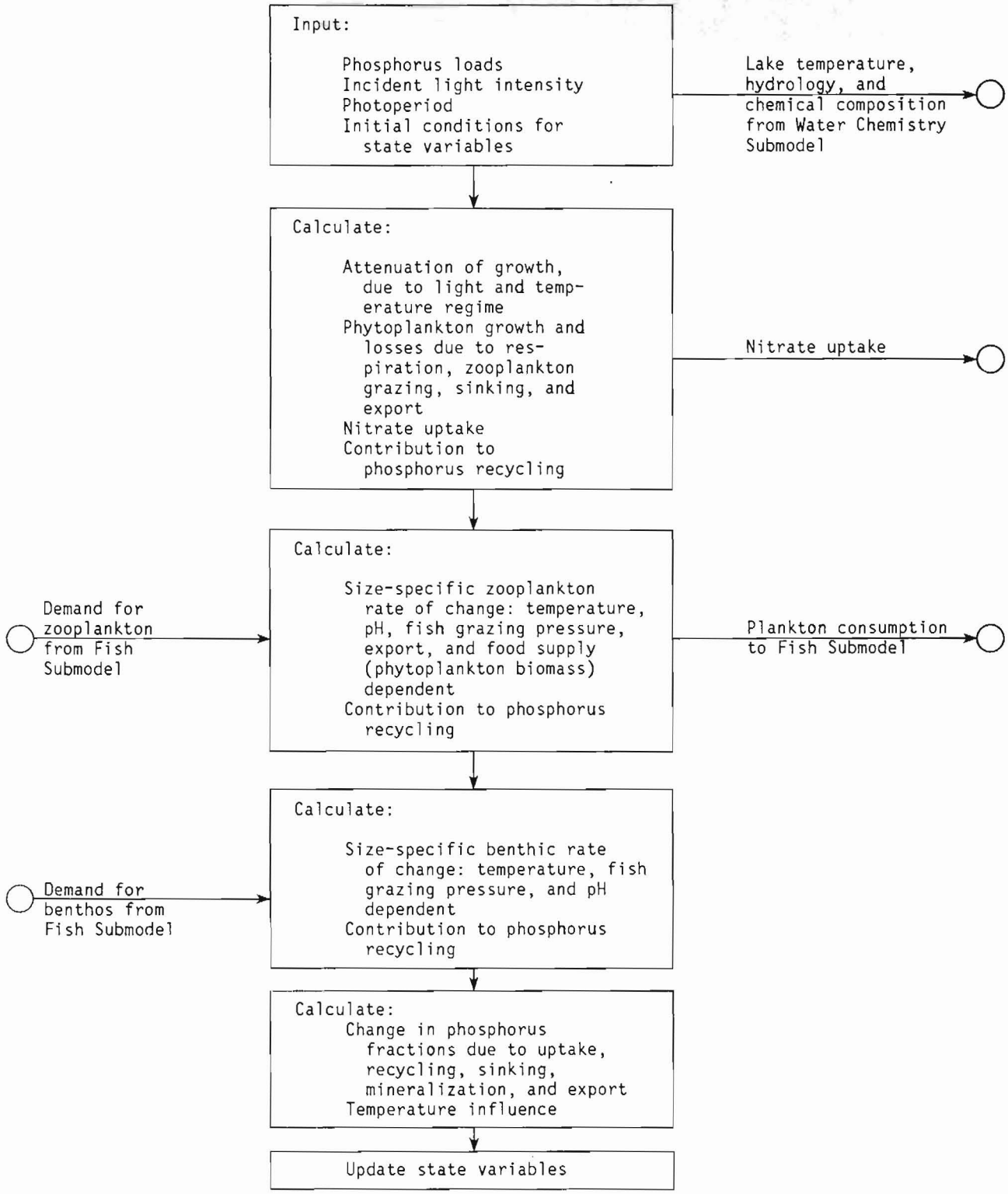


Figure 10. Calculation sequence for the lacustrine Plankton-Benthos Submodel.

One such relationship is the morphoedaphic Index (MEI) (Ryder et al. 1974). The MEI is calculated by dividing total dissolved solids (TDS) or conductivity by average lake depth. This index is significantly correlated with fish yield in a number of lakes. The requirement for using the MEI to predict fish yields in lakes are that the lakes be generally similar to those used in the regression analysis in terms of climate, flushing rate, and chemistry (Ryder et al. 1974). The regressions derived by Ryder et al. (1974) are for a variety of North American temperate lakes ranging in size from Lake Superior (82,414 km^2) to a small lake of only 2.6 km^2.

Using the MEI to predict fish growth requires several assumptions and approximations which limit the accuracy of the predictions. The prediction of fish yield from the MEI, while based on a significant regression, is only a rough estimate. Uncertainty about lake comparability decreases the reliability. The conversion of fish yield, which assumes moderate to intensive fishing effort, to fish growth is even more approximate. This conversion is made by assuming that fish yield in grams carbon (gC) is equivalent to fish growth potential in gC and that the potential annual food supply to support fish growth is distributed throughout the year according to the demand schedule demonstrated by the fish population when food is not limiting.

The formula produced reasonable estimates of fish growth, even though there were several reasons to question the results from this approach. This formulation might be adequate for some potential applications of the overall model. However, it is not as appropriate for developing research strategies as more detailed representations and will not be discussed further.

Filson Creek

The submodel structure developed to provide information on the food source for fish in the Harp Lake application did not seem suitable for application to Filson Creek because of the differences in trophic dynamics between lacustrine and lotic ecosystems. An existing lotic ecosystem model (Colby and McIntire 1978; McIntire and Colby 1978) was adapted and reparameterized for Filson Creek to the extent possible with existing data. Little information on biological processes was available for the stream ecosystem at Filson Creek.

The resulting model provides a logical structure for considering trophic support of fish in a lotic system, such as Filson Creek, even though it has limited usefulness for quantitative prediction.

The food base for fish is developed from both a detrital food chain (allochthonous) and a food chain driven by stream bottom algae (autotrophic process). The dynamics of the detrital food chain depend primarily on the seasonal schedule of allochthonous inputs from the adjacent terrestrial system. Autotrophic inputs are represented as the response of benthic algae to inputs of light and nutrients. The influence of acidity can be expressed through direct toxic effects on functional groups of primary consumers; i.e., the processes of both allochthonous and autochthonous inputs. Indirect effects of pH and nutrient concentrations (especially nitrates) can be expressed as changes in the rate of primary production.

The output of the lotic Plankton-Benthos Submodel includes the intermediate state variables of periphyton biomass; detrital components divided into large particle organic material (LPOM), conditioned large particle organic material (CLPOM), and fine particle organic material (FPOM); and the primary consumer functional groups. LPOM is defined as detrital particles larger than 1 mm in diameter; FPOM includes particles ≤ 1 mm. CLPOM is the portion of LPOM that has been exposed to the conditioning effects of microbial processes for the time period necessary before utilization by the stream detritus consumers. Consumer functional groups historically have been designated as shredders, collectors, and grazers, and that practice has been followed here. Periphyton is the food resource for the grazers, whereas shredders and collectors utilize CLPOM and FPOM, respectively.

Seven state variables are simulated. Four of these, the periphyton, shredders, collectors, and grazers, represent living functional groups; the other three (LPOM, CLPOM, and FPOM) are categories of detrital resources. The model structure is based primarily on current concepts of functional groups in stream ecology (e.g., Cummins 1974) and on the lotic ecosystem model developed by McIntire and Colby (1978). This ecosystem model reflects the modeling approach of Overton (1972, 1975), based on the general systems theory of Klir (1969). The current version of the lotic submodel is similar to the McIntire

and Colby model, but is also structurally similar to the Plankton-Benthos Submodel for lakes, presented in the previous section. The principal modifications include:

(1) A reduction in the number of detrital compartments from five to three;

(2) The deletion of the invertebrate predator functional group;

(3) The replacement of the vertebrate predator functional group by a coupling with the Fish Submodel;

(4) The incorporation of functions that represent toxic effects of acidity on the consumer functional groups; and

(5) Simplification of the calculation of stream hydrobiological characteristics.

The basic calculation sequence for the lotic Plankton-Benthos Submodel is illustrated in Figure 11. Difference equations for each functional group are:

Δ grazer biomass / Δ time = periphyton assimilation - respiration - emergence loss - fish predation (35)

Δ shredder biomass / Δ time - CLPOM assimilation - respiration - emergence loss - fish predation (36)

Δ collector biomass / Δ time = FPOM assimilation - respiration - emergence loss - fish predation (37)

Δ periphyton biomass / Δ time = gross primary production - respiration - particulate export - dissolved organic leaching - consumption by grazers (38)

Δ FPOM / Δ time = FPOM input from grazers, shredders, and collectors + FPOM input from fish + mechanical FPOM input - decomposition - export - consumption by collectors (39)

Δ LPOM / Δ time = LPOM input from terrestrial environment and from upstream - decomposition - export - transfer to CLPOM (40)

Δ CLPOM / Δ time = CLPOM input from LPOM - decomposition - export - consumption by shredders (41)

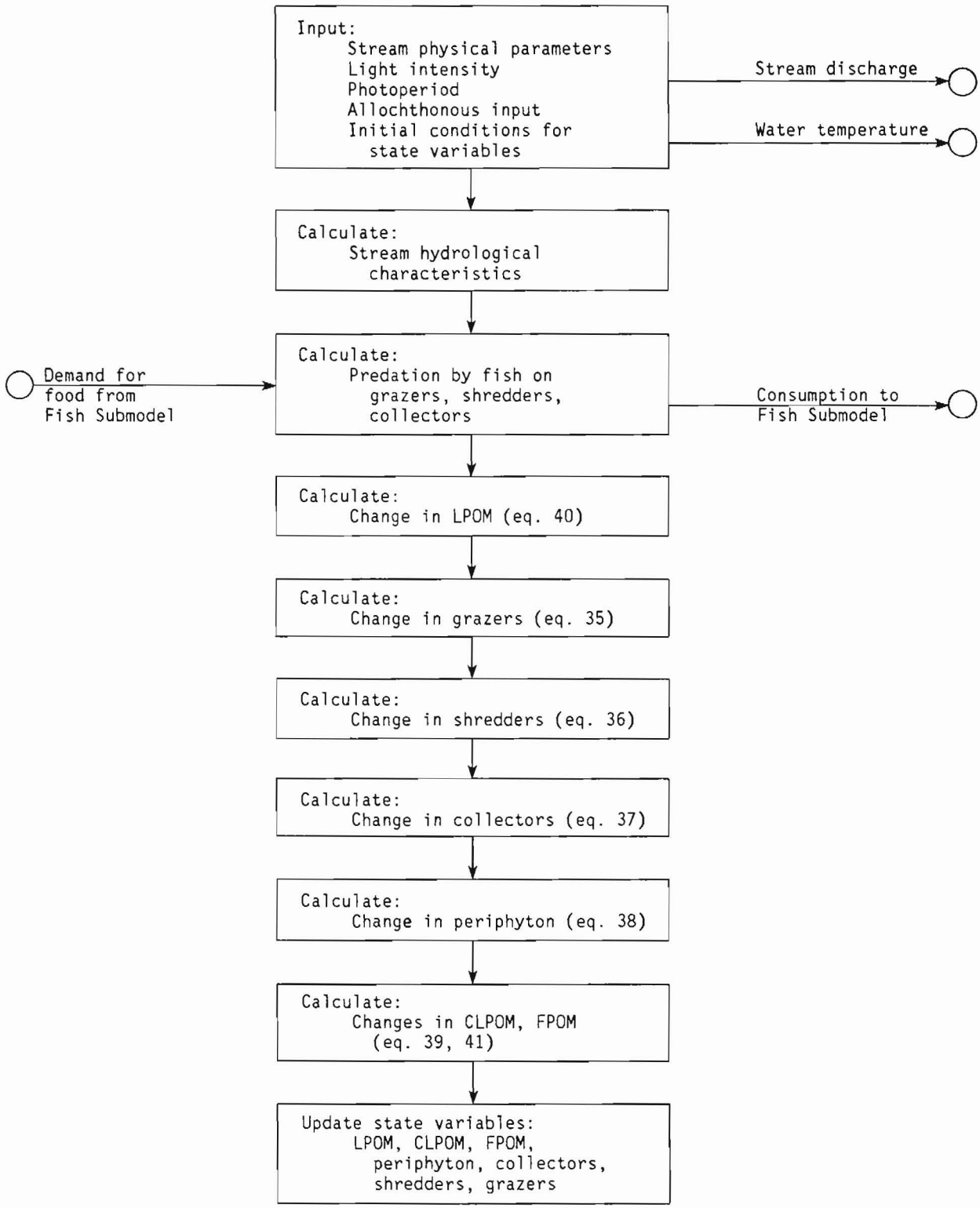


Figure 11. Calculation sequence for the lotic Plankton-Benthos Submodel.

The lotic Plankton-Benthos Submodel operates on a daily time step with output and connection with other submodels on a weekly time step.

COMPUTATIONAL APPROACH AND PARAMETER ESTIMATES

Harp Lake

The physical, chemical, and biological variables which influence the behavior of the detailed, lacustrine Plankton-Benthos Submodel are discussed below.

Phosphorus. Phosphorus is assumed to be the limiting nutrient for the biological compartments. Therefore, other macronutrients, such as nitrogen and carbon, are not explicitly modeled. The possibility of nitrate limitation following reductions in anthropogenic emissions of nitrogen oxides was discussed but not incorporated in the Plankton-Benthos Submodel. However, a number of contemporary models consider nitrogen limitation (e.g., Bierman et al. 1980; Rodgers and Salisbury 1981). Carbon limitation of phytoplankton growth was considered unlikely, even though total inorganic carbon levels are very low in many acidified lakes.

The total phosphorus within the water column is divided into two components, available and unavailable phosphorus. This recognizes the fact that uptake and utilization of phosphorus are limited to phosphorus fractions that can pass through the cellular membrane. Operationally, this means simulating two phosphorus pools, with phosphorus data input for each pool. Dissolved phosphorus values were assumed to represent available phosphorus, unavailable phosphorus was calculated as the difference between total phosphorus and available phosphorus.

Phosphorus amounts in the water column control the growth cycle of phytoplankton and, ultimately, the dynamics of the entire food chain. Other chemical or physical components may also influence the food chain. The kinetics of phosphorus are primarily concerned with simulating phosphorus recycling. This cycle conceptually describes the transformation of phosphorus

from unavailable forms to available forms. This transformation, referred to as mineralization, is parameterized as a first order temperature-dependent term. The mathematical formulation of mineralization used is:

$$R = K_r * P_u * \theta_R^{(T-20)} \tag{42}$$

where $R = \Delta$ unavailable phosphorus (mgP/l/day)

K_r = specific mineralization rate of unavailable to available phosphorus at 20°C (0.01/day)

P_u = unavailable phosphorus (mgP/l)

θ_R = Arrhenius coefficient describing temperature dependent function (1.08)

T = ambient temperature (°C)

Phytoplankton and zooplankton components contribute to the unavailable phosphorus pool through respiration and death. Release of phosphorus from phytoplankton is divided into unavailable and available phosphorus pools, in proportion to known internal storage pools. Unavailable phosphorus is also subject to settling from the water column.

The available phosphorus pool is the limiting nutrient source for phytoplankton, and biological depletion of available phosphorus reflects phytoplankton growth. A stoichiometric ratio between chlorophyll-a (indicator of phytoplankton biomass) and phosphorus is used to account for uptake of available phosphorus. Stoichiometric ratios for carbon and nitrogen to chlorophyll-a are also used, so that all changes are accounted for concurrently regardless of which nutrient is simulated.

Phytoplankton. Primary production is represented by a single phytoplankton compartment, even though phytoplankton simulation models can model specific functional groups of phytoplankton (Bierman et al. 1980). This additional complexity was considered inappropriate at this stage of model development. The change in the amount of phytoplankton is conceptually represented as

growth minus losses due to respiration, natural mortality, and zooplankton grazing. Phytoplankton growth and respiration/death are described below; grazing kinetics are discussed in the zooplankton subsection.

Growth of phytoplankton is represented as a first order process in which the maximum growth rate is attenuated by ambient temperature, light, and available phosphorus regimes. The specific growth rate, G_A, is formulated as:

$$G_A = K_A * \theta_A^{(T-20)} * F(L) * F(P_a) \tag{43}$$

where K_A = growth rate at 20°C (3.6/day)

θ_A = Arrhenius coefficient describing temperature dependent function (1.06)

T = ambient water temperature (°C)

Functions describing growth attenuation due to light (L) and available phosphorus (P_a) are also included in equation 43. The influence of these factors has been discussed in detail by DiToro and Matystik (1980).

Light influences growth in all photosynthetic communities. Steele (1965) formulated a relationship between maximum productivity, light saturation intensity, specific productivity, and specific light intensity. The depth integrated form of this equation (DiToro and Matystik 1980) is:

$$f(L) = \frac{e * f}{K_e * H} * [e^{-\alpha_H} - e^{-\alpha_o}] \tag{44}$$

where f = daily photoperiod (fraction of day)

K_e = light extinction coefficient (/m)

H = lake depth (m)

α_o = mean daily incident light/saturating light intensity

$$\alpha_H = \alpha_o * e^{-K_e H}$$

The light extinction coefficient (K_e) is calculated according to an empirical relationship which includes phytoplankton self-shading and lake color (P. Rodgers, DePaul University, EPA-LLRS, Grosse Ile, MI; personal communication). Sufficient data from lakes to represent accurately the functional influence of lake color was unavailable, and general assumptions were made. Mean daily incident light intensity is reduced when ice cover is present.

Attenuation of phytoplankton growth due to phosphorus limitation is formulated as a Monod function, dependent on external nutrient concentration:

$$f(P_a) = \frac{P_a}{K_s + P_a} \tag{45}$$

where K_s = half-saturation coefficient (0.005 mg P/l)

P_a = available phosphorus (mgP/l)

This saturation function represents the relationship between growth rate and external phosphorus concentration.

Respiration of phytoplankton is conceptually viewed as the sum of endogenous respiration and biomass losses as mediated by bacterial metabolic activity. This term is also a first order temperature dependent function. The specific formulation is:

$$D_A = K_D * \theta_D^{T-20} \tag{46}$$

where D_A = specific first order loss rate (/day)

K_D = specific loss rate at 20°C (.015/day)

θ_D = Arrhenius coefficient (1.08)

T = ambient water temperature (°C)

These losses result in additions to the phosphorus pools. Respiration losses are limited when standing stock reaches a lower bound that represents overwintering populations. Phytoplankton biomass is also subject to sinking from the water column and export via lake outflow.

Zooplankton. Two zooplankton compartments are represented, which differ only in terms of size-specific predation by fish. The relative contribution of these compartments to nutrient (phosphorus) recycling differ because their standing crops change at different rates according to differences in fish predation pressure. Zooplankton growth rate in each size compartment is dependent on the following kinetic interactions:

(1) Assimilation of phytoplankton (A_Z):

$$A_Z = G_Z * \frac{T}{20} * \frac{K_{AL}}{K_{AL} + AL} * \Phi \tag{47}$$

where G_Z = zooplankton specific grazing rate at 20°C (1.5/day)

K = a half-saturation constant for grazing rate versus food concentration (0.1 mgC/l)

AL = food concentration expressed as phytoplankton biomass (mgC/l)

T = ambient water temperature (°C)

Φ = assimilation efficiency of phytoplankton biomass by zooplankton (0.6)

(2) Respiratory loss rate (R_Z):

$$R_Z = K_Z * \theta_Z^{(T-20)} \tag{48}$$

where K_Z = zooplankton specific respiration rate at 20°C (0.025/day)

θ_Z = Arrhenius coefficient of temperature dependence (1.06)

T = ambient water temperature (°C)

Respiratory losses are limited when populations reach a lower bound by a formulation similar to that used for phytoplankton overwintering.

(3) Acidity. Empirical information relating pH to zooplankton assimilation (A_Z) and respiration (R_Z) are not available. Nevertheless, this submodel incorporates a relationship which recognizes the fact that zooplankton survival declines below a threshold pH value of 5.0 (Fig. 12). This function is intended to account for sources of zooplankton mortality other than fish predation and lack of food. The direct impacts of acidity and mobilization of heavy metals, and their interactions, for example, are implicitly represented by this formulation, as are acid-induced physiological imbalances in sodium, calcium, and other elements. It is assumed that growth rates are adversely affected by acidity at a pH threshold of 5.5 (Fig. 13). These values and the general form of the functional response were based on extrapolations from data on the effect of pH on fish.

Losses due to the size-specific demand for zooplankton as a food source indicated by the Fish Submodel reduce total zooplankton biomass in the lake. The basic formulations for dependency of zooplankton grazing rates on temperature and food supply and the dependency of respiration on temperature are from DiToro and Matystik (1980) and have been confirmed by experimental data (Hargis 1977). An algal refugium term was added to the grazing formulation to further limit grazing at low biomasses of algae and increase the numerical stability of the model. Reported values for assimilation efficiency vary widely (10-90%); however, the 60% figure used in this submodel is a reasonable estimate (Hargis 1977).

Phytoplankton are assumed to be the principal food source for zooplankton, although bacteria and detritus provide some nutrition. The grazing rate function is applied to both zooplankton size compartments and treats all phytoplankton the same, regardless of the size, shape, or "palatability" of individual phytoplankton species. There is abundant evidence for food size

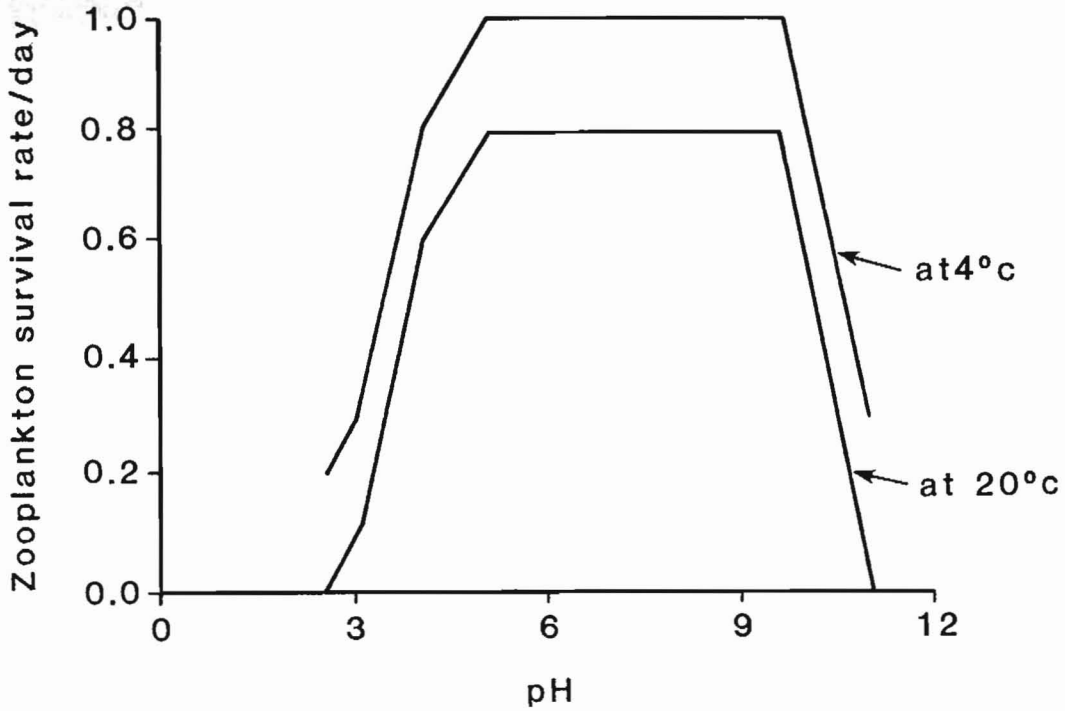


Figure 12. Temperature and pH effects on zooplankton survival.

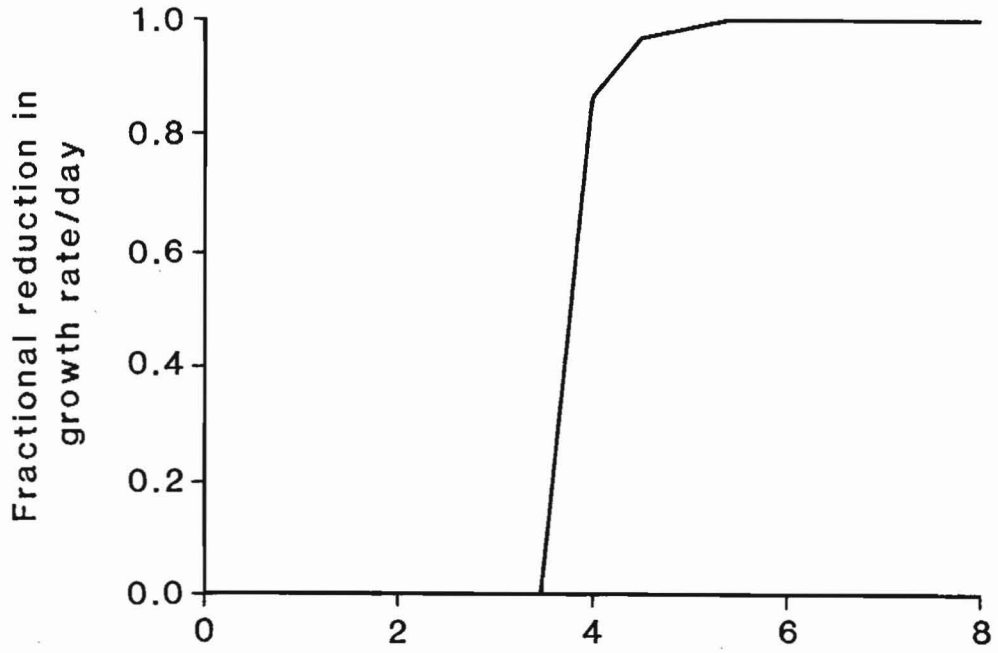


Figure 13. pH limitation of zooplankton and benthos growth.

selection by zooplankton and differential ingestion and assimilation efficiences by zooplankton that are fed various phytoplankton taxa (literature reviewed by Hargis 1977). However, a single average grazing rate should be applied until changes in phytoplankton species composition in response to increased acidity is documented. There is also justification for introducing different maximum grazing rates for small and large zooplankton as a refinement to the submodel (Parsons and Takahashi 1973).

Benthos. Two benthic compartments, based on size class, are treated in the submodel in the same manner as the zooplankton. These two compartments behave identically except for size-specific fish predation. The kinetic representation for benthos respiration follows the formulation described for zooplankton. The equation was simplified so that export of benthos (assumed to be negligible) and food limitation factors were not included. In contrast to the zooplankton formulation (eq. 35), growth of benthos is not modeled dynamically. Figures 13, 14, and 15 represent pH-related growth limitations of benthos, temperature dependence of benthic growth, and effects of acidity on benthic survival, respectively. The biomass of benthic organisms entering the lake via stream flow is assumd to be balanced by the biomass that exits via the lake outlet (i.e., net export of benthos = 0).

Filson Creek

Computational approach and parameter estimates follow McIntire and Colby (1978) and the more detailed documentation of Colby and McIntire (1978), with the following adaptations for the Filson Creek application.

Hydrology. Insufficient field data were available to express stream depth, width, and cross sectional area as power functions of discharge or to estimate the Manning roughness coefficient by curve fitting as was done for the original model application to Oak Creek, Oregon (Colby and McIntire 1978). The Manning equation for discharge (Bovee and Milhous 1978)

$$Q = (1.486/n) * R^{2/3} * S^{1/2} * A \qquad (49)$$

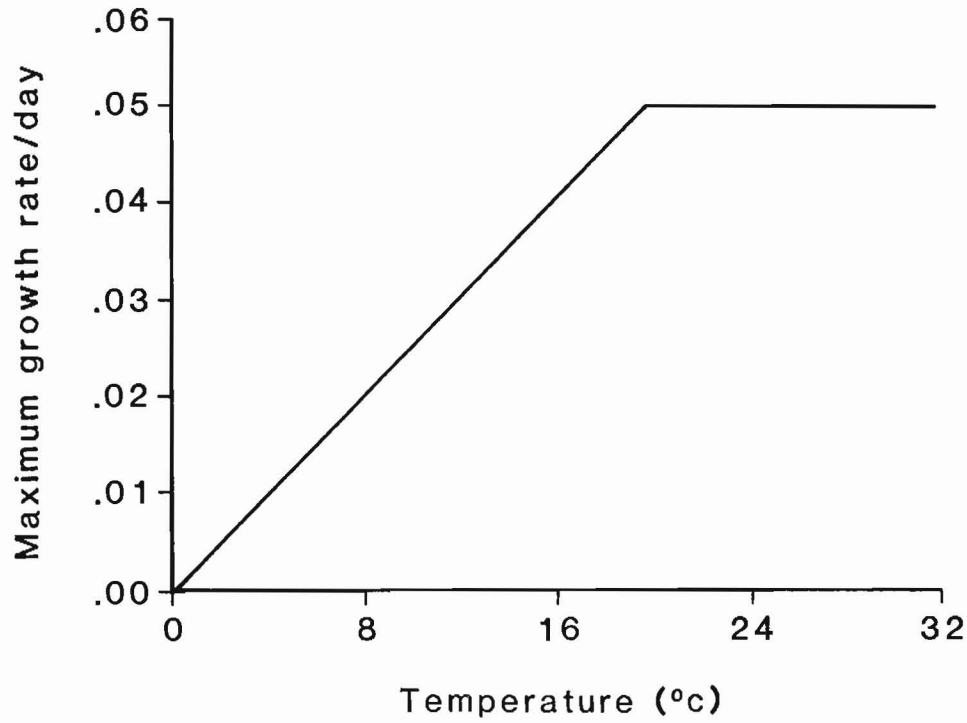


Figure 14. Maximum potential benthic growth rate.

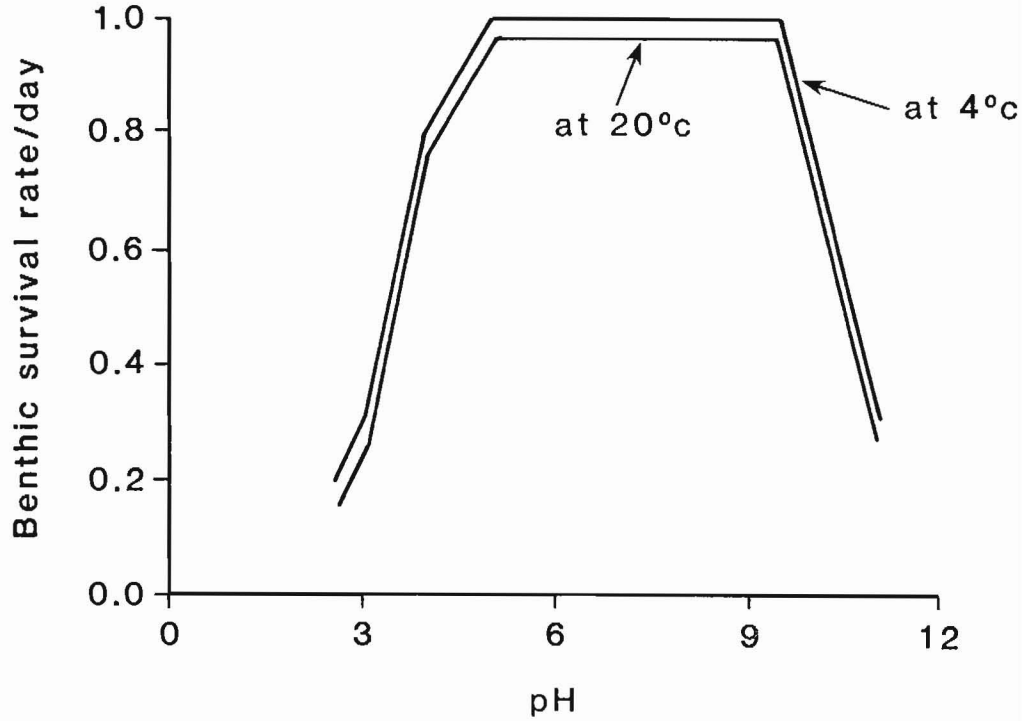


Figure 15. Temperature and pH effects on benthic survival.

where Q = discharge (ft^3/sec)

R = hydraulic radius (ft)

S = slope

n = Manning roughness coefficient

A = cross sectional area (ft^2)

was solved for the required hydrological parameters as a function of discharge by assuming a constant Manning roughness coefficient, a constant channel depth to width ratio, and utilizing a value for slope estimated from topographic maps of the Filson Creek area.

Detrital components. The four large particulate organic matter compartments of McIntire and Colby (1978) were condensed to two. Fast and slow large particulate organic matter (FLPOM and SLPOM) and fast and slow conditioned large particulate organic matter (CFLPOM and CSLPOM) were represented by the compartments large particulate organic matter (LPOM) and conditioned large particulate organic matter (CLPOM). A 100-day conditioning lag was used to convert LPOM to CLPOM, with a decomposition-respiratory loss parameter intermediate between that of McIntire and Colby's (1978) fast and slow compartments.

Forcing functions. The model assumes that nitrate limits primary production. The submodel was, therefore, coupled to nitrate concentrations provided by the Water Chemistry Submodel. Water temperature values were determined from data for Filson Creek in 1978-1979. The Version I hypothetical light schedule of McIntire and Colby (1978) was utilized. In the absence of actual data from Filson Creek, an allochthonous input schedule was hypothesized to provide 216 g dry weight/yr of LPOM, with high daily rates in the fall. Accurate measurements of the energy input schedules of both light and organic materials would be necessary to more adequately parameterize this model to Filson Creek.

Predation. Invertebrate predation is not represented in the model and vertebrate predation is replaced by a coupling with the Fish Submodel. The Fish Submodel provides a demand for food, and the fraction of this demand

which could be met is calculated by McIntire and Colby's (1978) formulation modified to exclude competition with invertebrate predation and partitioned among grazers, shredders, and collectors according to their relative biomass.

Parameter changes. Several additional parameter adjustments were made from the documentation of Colby and McIntire (1978). The respiration parameter for shredders and collectors was set at 0.022, rather than 0.0296 and 0.0146. A constant light extinction coefficient was used, rather than a coefficient that was a function of suspended load, because of the lack of information on suspended load.

Acidity. Little information is available to formulate the functional response of aggregated, process-defined components, such as those utilized in this conceptual approach to stream ecosystems, to acidity. Species elimination, species replacements, or shifts in relative species importance may or may not imply a change in the overall behavior of the subsystem or its connection to other subsystems, such as fish. To illustrate how such functional responses might be incorporated into this process-oriented conceptualization, some of the pH relationships utilized in the lacustrine Plankton-Benthos Submodel were applied to the processes of feeding (using the shape of the curve of Fig. 13 at 4° C) and respiration (using the shape of the curve of Fig. 12) of grazers, shredders, and collectors.

Chapter Authors: Paul Rodgers, DePaul University, EPA-LLRS; Jack Hargis, University of Minnesota; C. David McIntire, Oregon State University; Richard Miller, The Institute of Ecology; Gregor Auble, FWS; David Marmorek, Environmental and Systems Analysis, Ltd.

Chapter Contributors (in alphabetical order): Ken Biesinger; EPA; Dave Brakke, Western Washington University; Lee Conway, Brookhaven National Laboratory; William Kovalak, Detroit Edison; Charles Powers, EPA; Tom Roush, EPA.

7. FISH SUBMODEL

SCOPE

The Fish Submodel is designed to predict the impact of lake and stream acidification on the dynamics of brook trout and white sucker populations. The submodel provides a framework for integrating both direct stress effects, such as pH and metal-induced mortality, and indirect stress effects, such as reduction in forage base.

Processes represented by the Fish Submodel are linked to the other submodels through the transfer of information about available food (in size classes < 1 mm and ≥ 1 mm) and the ambient chemical environment. Limited food supplies (Plankton-Benthos Submodel) can result in reduced growth or direct mortality. The ambient chemical environment can result in fish mortality because of the toxicity of inorganic aluminum and hydrogen ion concentrations. The Fish Submodel has no other direct submodel links. Changes in aquatic chemistry resulting from changes in fish populations are hypothesized to occur indirectly through fish predation on the plankton-benthos communities.

The Fish Submodel is designed to reflect the underlying mechanisms that govern populations in stressed systems. That is, the model simulates the logical consequences of management actions and facilitates testing of alternative hypotheses about the structure and function of the system. The adequacy of the hypotheses can be tested by comparing predicted outcomes with observed conditions. In addition, hypotheses about the system can be developed and tested in field and laboratory research programs.

MODEL APPROACH

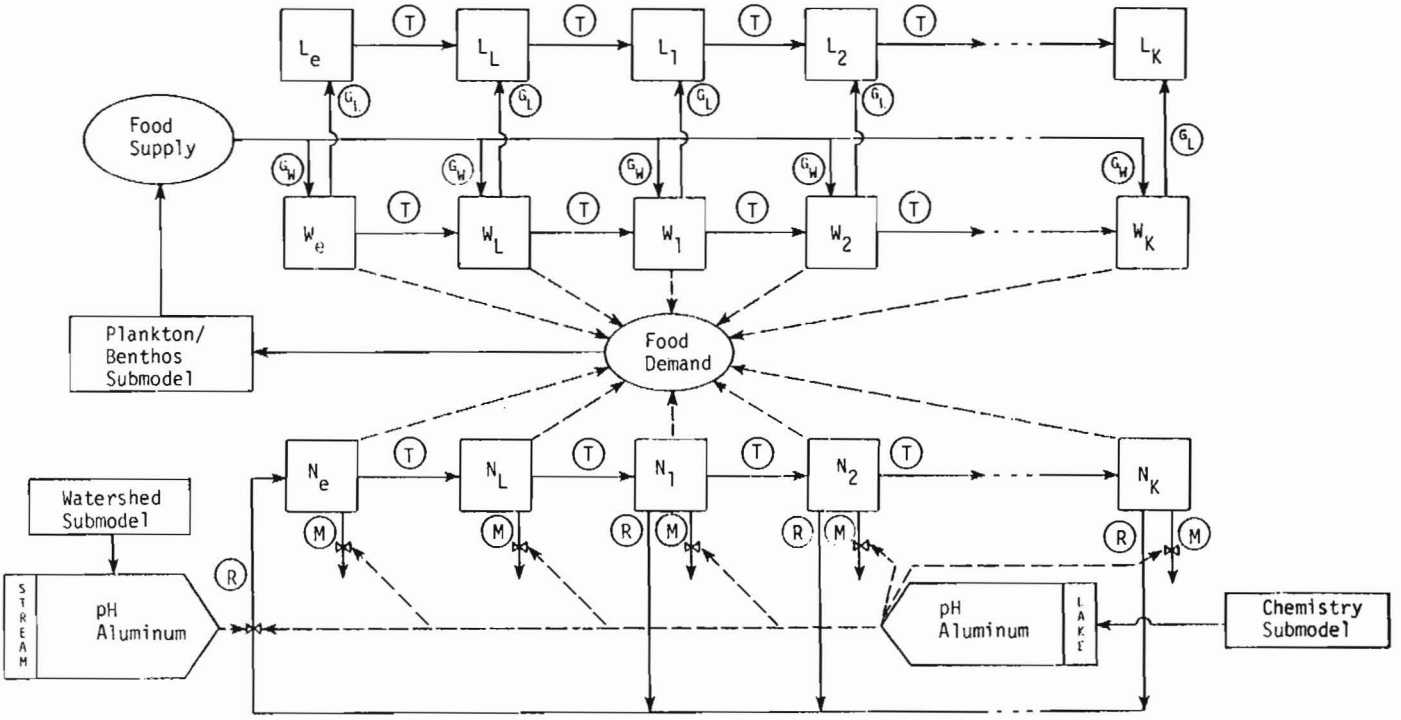
The primary state variables for the Fish Submodel are mean weight, mean length, and number of individuals by life stage. These three variable sets are believed to be the minimum amount of data needed in order to meet model

expectations. Each fish population is divided into life stages based on differences in food requirements and resistance to pH and aluminum stress. Although acidification effects tend to be gradual, they can be highly variable over time and space and have a crucial bearing on the continued existence of fish populations. For this reason, a conceptually simpler model was not acceptable. Brook trout and white suckers were chosen as representative fish species of aquatic systems susceptible to acidification. Other fish species may also be important from economic, recreation, and ecological viewpoints. Brook trout and white suckers represent a compromise between considering all of the important species and only those species for which there is adequate available information. Other species, particularly cyprinids, can be included in the model as additional information becomes available.

An overview of the Fish Submodel is presented in Figure 16. This submodel may be considered as a highly modified Leslie matrix model (Leslie 1945). Individuals are lost from the system through natural or chemically-induced mortality. Individuals are added to the system through reproduction, which can occur in both the lake and stream subsystems. Food requirements depend on the number of fish present, their average weight, and the amount of food that can be utilized per individual. The amount of food actually available is determined by the Plankton-Benthos Submodel.

Fish grow at their maximum rate when individuals receive all the food they can consume during each life stage. The rate of growth declines as food becomes limited. The different ability of the various life stages to acquire food is not incorporated into the Fish Submodel. However, zooplankton is divided into size classes of less than and greater than 1 mm, to take into consideration the fact that food may be limiting to adult fish and not limiting to ichthyoplankton or vice versa.

The available food is converted to a corresponding increase in average biomass for each cohort. This conversion is based on an empirical description of the relationship between the instantaneous rate of growth and the maximum age-specific growth rate, the fraction of the maximum amount of food that is actually received, and the amount of food required for maintenance. The



State Variable Definitions

L_i = average length of life stage i (mm)

W_i = average weight of life stage i (g)

N_i = number of individuals of life stage i

Process Definitions

G_L = growth in length

G_W = growth in weight

M = mortality

R = reproduction

T = transfers between life stages, governed by time only

= control

Figure 16. State variables and processes in the Fish Submodel and their connections with other submodels. The same structure is applied to both brook trout and white suckers. Example is for species with k life stages.

increase in average length for individuals in each life stage is dependent on changes in weight. If the weight change is positive, the length increment is governed by the allometric relation between length and weight. If the weight change is negative, no change in length occurs.

A more complex model than that presented in Figure 16, linking traditional fisheries approaches with bioenergetics models, would be desirable as a fish submodel. However, our understanding of how pH and aluminum concentrations alter the amount of energy available for growth and reproduction is too incomplete to support such a model at this time. The current model structure is a compromise between desirable model complexity and limited available data.

COMPUTATIONAL APPROACH AND PARAMETER ESTIMATES

The Fish Submodel (Fig. 16) can be expressed as a series of general functional expressions:

Number of eggs produced	= f_1	(Numbers and average weights of all reproductive life stages, pH and aluminum-induced mortality)	(50)
Number of individuals in life stage i at time t+1	= f_2	(Number of individuals in life stage i at time t, natural survival rates, pH and aluminum-induced mortality)	(51)
Average weight of individuals in life stage i at time t + 1	= f_3	(Average weight of individuals of life stage i at time t, age of fish, maximum growth rate, fraction of maximum ration received)	(52)
Average length of individual of life stage i at time t + 1	= f_4	(Average length of individuals of life stage i at time t, average weight increment of life stage i at time t + 1, allometric relation between length and weight)	(53)

Equations (50) through (53) are implemented as recursive relations with a time-step of 1 week. The discrete formulations of these equations permit the sequential calculation scheme outlined in Figure 17.

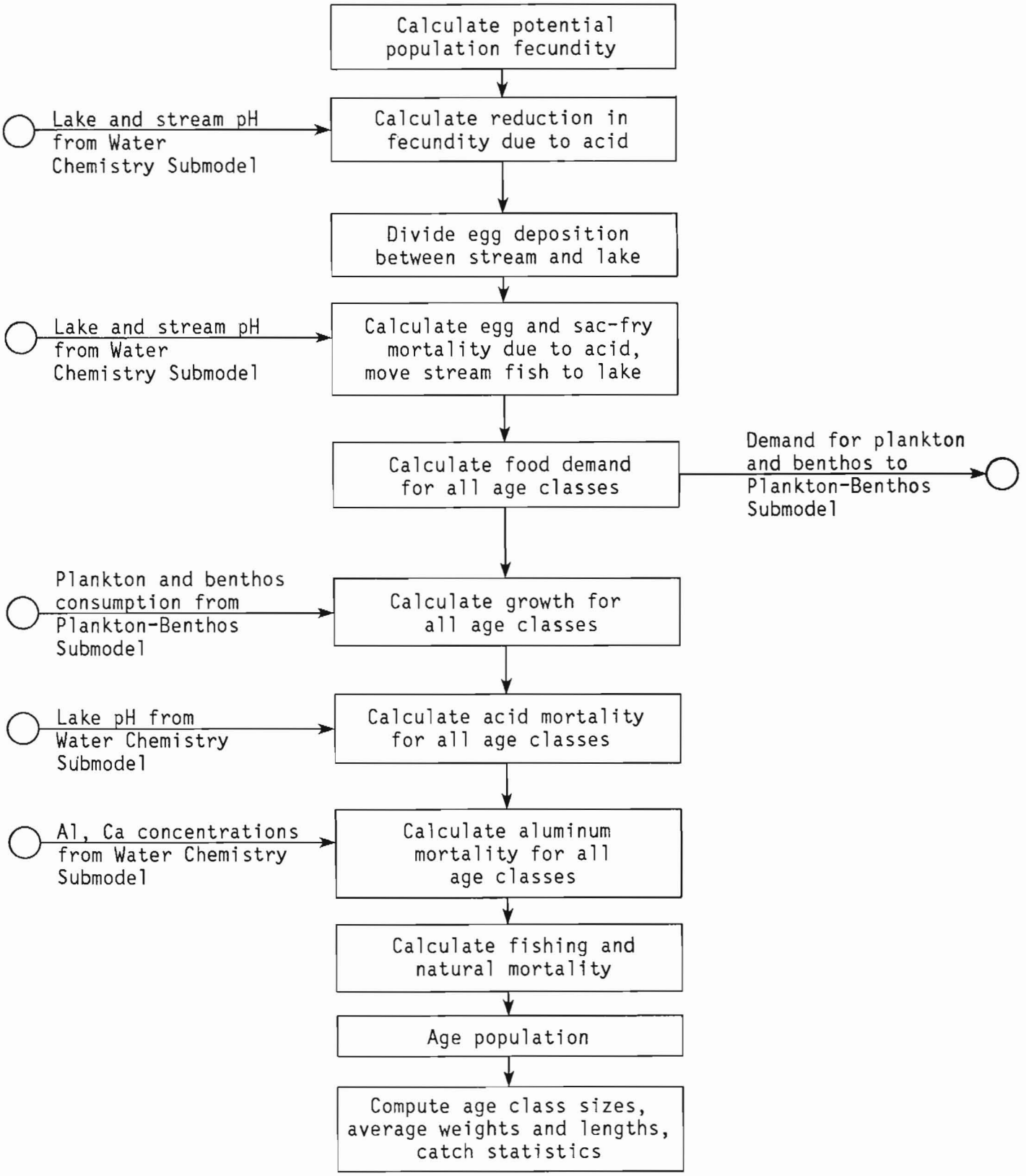


Figure 17. Calculation sequence for the Fish Submodel.

Reproduction

The number of eggs produced is a function of the number of mature individuals in each age class and their average fecundity, which is determined by average weight (brook trout) or average length (white sucker). Thus, fecundity is indirectly linked with food availability according to the equation:

$$E_t = \sum_{i=m}^{k} p_i * N_{i,t} * F_{i,t} \tag{54}$$

where E_t = number of eggs produced at time t

$N_{i,t}$ = number of individuals of age i at time t

$F_{i,t}$ = average fecundity of fish of age i at time t

$$F_{i,t} = g(W_{i,t}) \tag{55}$$

where $g(\bullet)$ = function relating fecundity to weight (grams)

$W_{i,t}$ = average weight of individuals of age i at time t.

A senescence factor (p_i) is used to reduce fecundity in white suckers over 8 years old (Fig. 18). The senescence factor was not applied to brook trout because populations are usually short lived and subject to intense fishing pressure in many lakes. The fecundity equation does not include the effect of chronic pH stress on egg production. Chronic pH stress has been observed to decrease egg production in laboratory studies (Ruby et al. 1978) and in one field study (Beamish 1976). There were insufficient data available to incorporate this effect into the model, even though selection for resistant individuals may eliminate the adverse effect of pH stress on reproduction in actual field conditions. Such selection would probably act rapidly on phenotypes, but much more slowly on genotypes.

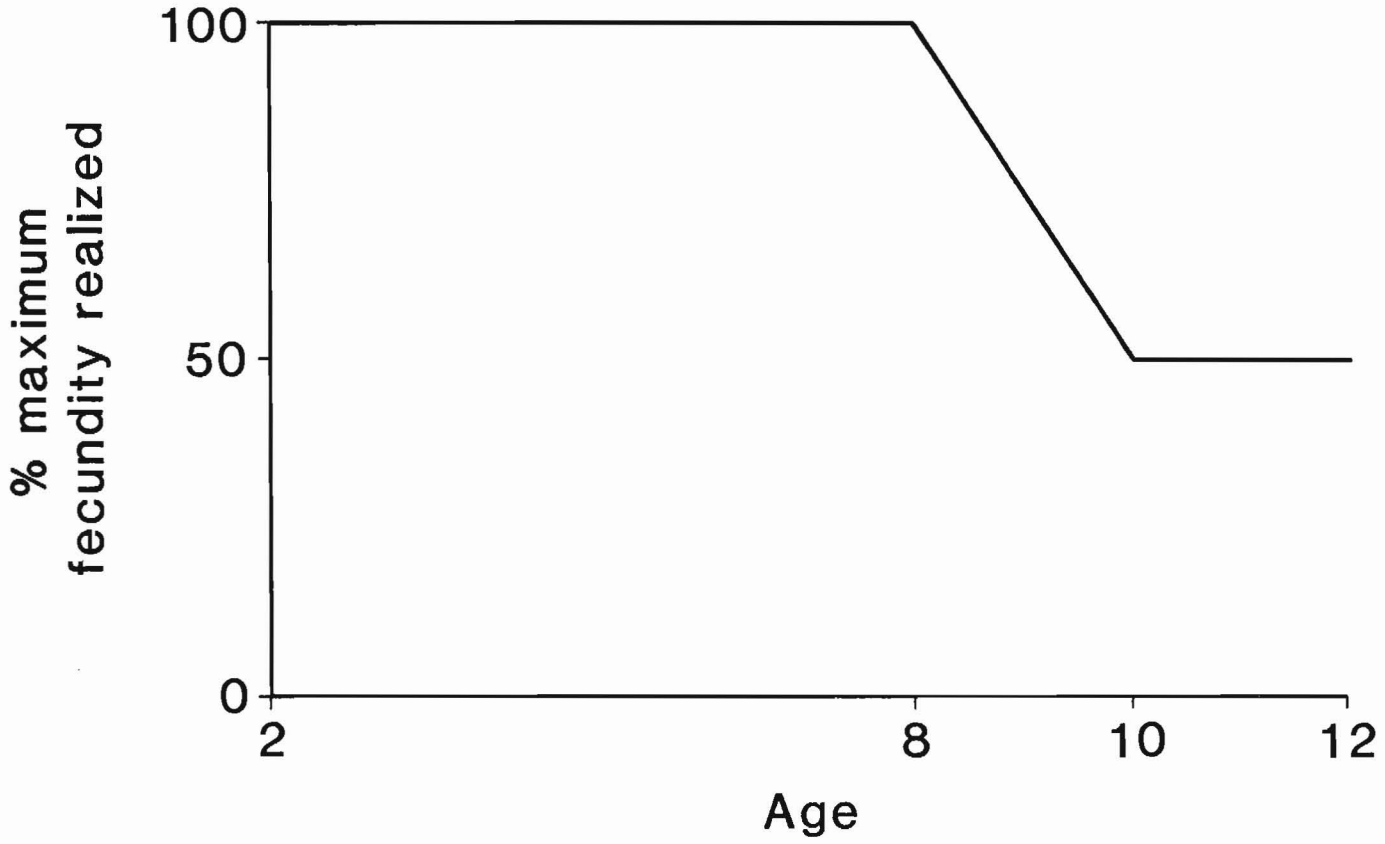


Figure 18. Percent of maximum fecundity realized as a function of age.

The functions g(•), which relate predicted egg production to average weight or length, are:

$$\text{brook trout:} \quad F_{i,t} = -111 + 5\ W_{i,t} \tag{56}$$

$$\text{white sucker:} \quad \log_{10} F_{i,t} = -1.88 + 2.47 \log_{10} L_{i,t}$$

where $L_{i,t}$ = estimated length (mm) of fish of age $_i$ at time t

The estimated length $L_{i,t}$ is derived from the inverse of the length-weight relationship for white suckers (see section on Growth in Length) and does not equal the actual $L_{i,t}$ state variable in the model. The estimated length $L_{i,t}$ is used to reduce fecundity by reducing the "effective" length of an age class whenever food limitations decrease weight.

Mortality

Brook trout and white sucker populations are subject to both natural mortality and stress-induced mortality resulting from concentrations of hydrogen ions and inorganic aluminum (Fritz 1980). The way that life stage mortalities are incorporated into this version of the model significantly differs from the approach resulting from the first Acid Precipitation Workshop. The original mortality rates were obtained by aggregating information on toxicity relationships from experiments described in the literature. Both chronic and shock effects were considered and mortality sources were assumed to act independently, resulting in highly improbable mortality rates. A recent dissertation from Cornell University (Baker 1981) summarizes mortality rates for brook trout and white suckers as a function of pH and aluminum acting together. Polynomial expressions, resulting from factorial experiments (Baker 1981), are used in this model. These equations are especially useful because the life stages tested closely corresponded to those used in the model and the duration of experiments (6 days) approximated the 7-day time-step in the model. Use of the equations from Baker (1981) provides a more realistic representation of pH and aluminum-induced mortalities than the results from the first Acid Precipitation Workshop.

The general form of the mortality function is:

$$Y = b_0 + b_1[Al_a] + b_2[H^+] + b_3[Al_a]^2 + b_4[H^+]^2 + b_5[H^+] * [Al_a] \quad (57)$$

where $Y = \log_e$ (number dying/number surviving)

$[Al_a]$ = concentration of inorganic aluminum (mg/l)

$[H^+]$ = concentration of hydrogen ions (moles/l)

b_i = least squares regression estimates

A stepwise procedure is used for the regression calculation, so that the value of $b_i = 0$ for some of the models. The regression models used are listed in Table 3. Regression models were developed for the following life stages for each species: eggs (from fertilization to the eyed stage); eggs (from the eyed stage to hatching); larvae (from hatching to swim-up); and older larvae (post swim-up). The value (Y) is back transformed to survival rate as follows:

$$S = 1 - (e^Y/(1+e^Y) \quad (58)$$

where S = survival fraction

Y = value obtained from equation (57)

The response functions do not directly consider acclimation or mortality resulting from chronic pH stress. Mortality from chronic pH and aluminum stress is considered minimal because acclimation to these stress factors appears to occur rapidly in lakes (Muniz and Leivestad 1981; Rahel and Magnuson 1981). Because pH and aluminum stress tend to remove sensitive individuals from the population rapidly, chronic effects are minimal. Little is known about the genetic implications of this effect. In this submodel, a cohort is assumed to become less sensitive to pH shocks as the total number of pH shocks experienced increases, and when the number of acute pH depressions exceeds eight, the cohort is resistent to further pH shocks, and no additional pH shock mortality is imposed (Guthrie 1981). The switching mechanism and acute

Table 3. Regression models relating hydrogen ion concentration (H^+ moles/l) and inorganic aluminum (Al_a mg/l) to mortality (Y) of early life history stages of brook trout (ST) and white suckers (WS) (after Baker 1981).

1) $$Y_{(ST\ eyed\ egg)} = -2.98 + 1.47 * 10^9 * [H]^2 + 1.39[Al_a] - 1.98 * 10^5 * [H] * [Al_a]$$

2) $$Y_{(WS\ eyed\ egg)} = -1.84 + 7.63 * 10^5 * [H] - 2.07 * 10^{10} * [H]^2 + 44.7[Al_a] - 57.6[Al_a]^2 - 8.4 * 10^6 * [H] * [Al_a] + 1.56 * 10^{11} * [H]^2 * [Al_a] + 9.71 * 10^6 * [H] * [Al_a]^2$$

3) $$Y_{(ST\ hatch)} = -2.89 + 1.62 * 10^9 * [H]^2 + 1.55\ [Al_a] - 2.04 * 10^5 * [H] * [Al_a]$$

4) $$Y_{(WS\ hatch)} = 1.36 + 6.83 * 10^5 * [H] - 1.81 * 10^{10} * [H]^2 + 106\ [Al_a] - 489[Al_a]^2 - 6.13 * 10^6 * [H] * [Al_a] - 2.70 * 10^{10} * [H]^2 * [Al_a] + 2.92 * 10^7 * [H] * [Al_a]^2$$

5) $$Y_{(ST\ sac\text{-}fry)} = -3.89 - 5.69 * 10^4 * [H] + 1.53 * 10^9 * [H]^2 + 19.6[Al_a] - 9.34 * 10^5 * [H] * [Al_a] + 1.18 * 10^{10} * [H]^2 * [Al_a]$$

6) $$Y_{(WS\ sac\text{-}fry)} = -2.80 + 3.13 * 10^5 * [H] + 34.7[Al_a] - 1.74 * 10^6 * [H] * [Al_a]$$

7) $$Y_{(ST\ swim\text{-}up)} = -3.59 + 2.02 * 10^3 * [H] + 17[Al_a] + 2.24 * 10^5 * [H] * [Al_a]$$

8) $$Y_{(WS\ swim\text{-}up)} = -2.90 + 1.04 * 10^5 * [H] + 46.1[Al_a] - 55.1[Al_a]^2 - 1.96 * 10^6 * [H] * [Al_a]^2$$

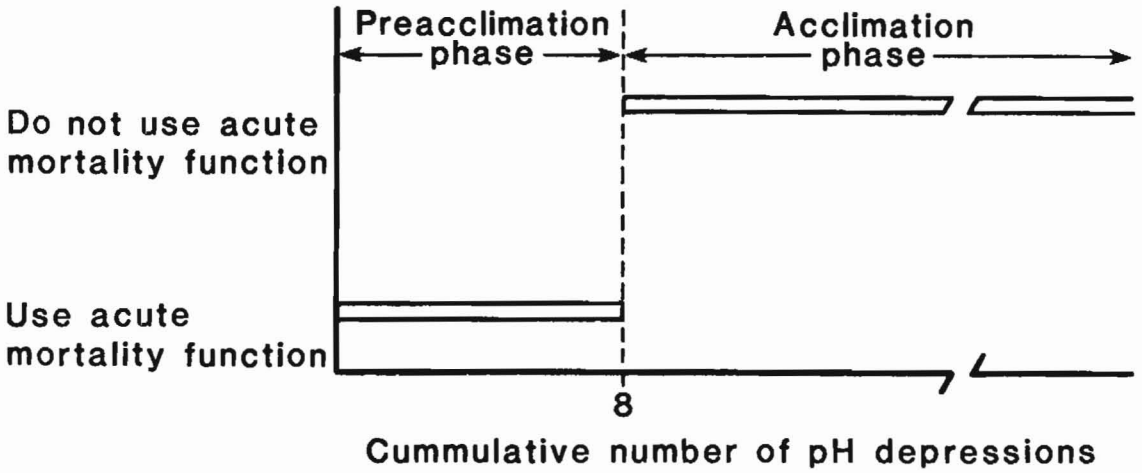
mortality function are illustrated in Figure 19. The total mortality that is imposed on a cohort durng the period it is susceptible to pH shocks is $1.0-0.85^4 \approx 48\%$. Complete mortality occurs whenever pH falls below 3.5 for brook trout or 4.2 for white suckers. This constraint is imposed because survival values derived from Baker's equations increase when pH declines below levels (i.e., 3.5 and 4.2) where Baker's equations were intended to be used. More complete discussions of pH and aluminum effects on fish are in Baker (in press) and Baker and Schofield (in press).

Calcium (Ca) ameliorates the effects of pH and aluminum whenever Ca concentrations exceed 2 mg/l (Leivestad and Muniz 1981). However, there was not sufficient time to incorporate this effect into the current model.

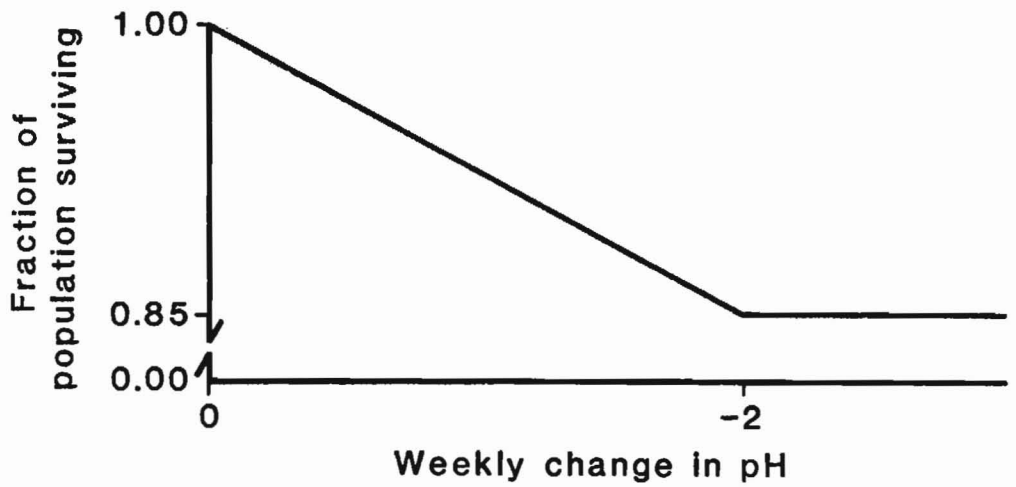
Natural mortality is difficult to include in the model because few field studies have measured mortality for all life stages. Nominal mortality rates were derived by assuming that populations were in equilibrium. Therefore, existing data, however incomplete, can be used to calculate the unknown mortality rates using a modified equivalent adult approach (Goodyear 1978). Briefly, this procedure assumes that population structure is in equilibrium and that birth and death rates are the same. The unknown mortality rate can be estimated if the birth rate and some mortality rates are known. Estimated mortality rates usually spanned several of the life stages included in the model, making it necessary to partition mortality according to assumptions about the fraction of the unknown mortality occurring in each life stage. The details of these assumptions are expressed as weekly survival rates for the age classes of each species (Table 4).

Table 4. Weekly age-specific survival rates for test populations of brook trout and white suckers.

	Survival rates by age class						
Species	0	1	2	3	4	5	6
Brook trout	.897	.981	.982	.982	-	-	-
White sucker	.626	.989	.989	.989	.989	.990	.949



(a) Acclimation function for each cohort of each species



(b) Acute mortality function for adults

Figure 19. Incorporation of acclimatization of adult fish to acute pH depression.

A common assumption in fisheries models is that sources of mortality tend to act independently of one another. Thus, instantaneous rates of mortality, such as $Z_1 \ldots Z_n$, are added to the model, with the exponential of the sum yielding the overall survival rate. However, a minor form of compensation is assumed to occur for this model. Decreases in fish numbers are assumed to be governed by the minimum survivorship value of the natural survival rate and the survival rate predicted from pH and aluminum stress. In summary, the actual survival rate used to change population numbers is defined as the lesser of the stress-induced mortality rate and the natural mortality rate.

In equation form, the number of individuals in each life stage are calculated as follows:

$$N_{i,t+1} = \min\,[S_1(pH, Al), S_2] * N_{i,t} \tag{59}$$

where $S_1(pH, Al)$ = survival rate as a function of pH and inorganic aluminum

S_2 = natural survival rate.

Equation (59) allows for partial compensation of total mortality because the base or a lower survival rate is always applied.

Growth in Weight

Average growth in weight is governed by the transfer of food from the Plankton-Benthos Submodel and the fish species and parameters specific to their life stages. The computational sequence calculates a total demand for food, sends this "request" to the Plankton-Benthos Submodel, and receives the total quantity of available food partitioned into sizes less than or greater than 1 mm. The quantity of food allocated to each age class is in proportion to the quantity demanded.

The total quantity of food demanded ($F_{d,t}$) is defined as:

$$F_{d,t} = \sum_{s=1}^{2} \sum_{i=1}^{k_s} RMAX_s(W_{i,t}) * N_{i,t} \tag{60}$$

where $RMAX_s(W_{i,t})$ = maximum ration (gC) that could be used by life stage i. The maximum ration is defined as 5% of the average weight ($W_{i,t}$) of life stage i at time t.

s = subscript relating to species

i = subscript for life stage

The value of $F_{d,t}$ is sent to the Plankton-Benthos Submodel and some fraction (from 0.0 to 1.0) of $F_{d,t}$ is supplied ($F_{s,t}$). The quantity $F_{s,t}$ is less than or equal to $F_{d,t}$. The actual ration allocated per individual ($R_{i,t}$) for each age class is:

$$R_{i,t} = \frac{F_{s,t}}{F_{d,t}} * RMAX_s(W_{i,t}) \tag{61}$$

The rate of change of average weight, as determined by the actual ration received, is calculated as:

$$\begin{aligned} W_{i,t+1} &= W_{i,t} + \Delta W \\ &= W_{i,t} + (e^G - 1) * W_{i,t} \end{aligned} \tag{62}$$

where $G = G_{max,i} * \sin\left(\frac{\pi}{2} * \frac{R-R_n}{R_m-R_n}\right)$

$G_{max,i}$ = maximum instantaneous rate of growth for life stage i

$R = R_{i,t}$ = actual ration allocated to life stage i

$R_m = RMAX_s(W_{i,t})$ = maximum ration for life stage i as a function of average weight

$R_n = RMN_s(W_{i,t})$ = maintenance ration for life stage i as a function of average weight. RMN_s was defined as 1.5% of $W_{i,t}$

The maintenance ration is set at 1.5% of body weight per day for modeling considerations. The equation for G (taken from Stauffer 1973, as described by Ricker 1979) directly links the traditional calculation of instantaneous growth rate with a more realistic bioenergetic approach. Figure 20 demonstrates the conversion of ration received to change in weight. If the maximum ration is received, growth in weight is at a maximum; if the ration equals maintenance, there is no growth; and if the ration falls below maintenance, there is a loss of weight. The translation of these ratios to realized growth in weight is shown in Figure 21.

The model does not consider many bioenergetic factors, particularly the dependence of metabolism on temperature. Future models should incorporate the effects of temperature, pH, and aluminum on the distribution of energy for maintenance, growth, and reproduction. The present model calculates fecundity as a function of mean weight only. There is considerable variation in reproductive activity among fish, particularly when subject to stress, and available energy for reproduction should be explicitly considered in the model.

Growth in Length

The rate of increase in length depends on the relative gain in weight and is computed according to the allometric relationship between length and weight. This relationship is usually defined in the fisheries literature as $W = aL^b$, where W = weight, L = length, and a and b are regression constants. Weight and length are both functions of time (age), and the rate of change in weight with respect to time is:

$$\frac{dW}{dt} = a * b * L^{b-1} * \frac{dL}{dt}$$

solving for dL/dt:

$$\frac{dL}{dt} = \frac{dW}{dt} * (a * b * L^{b-1})^{-1}$$

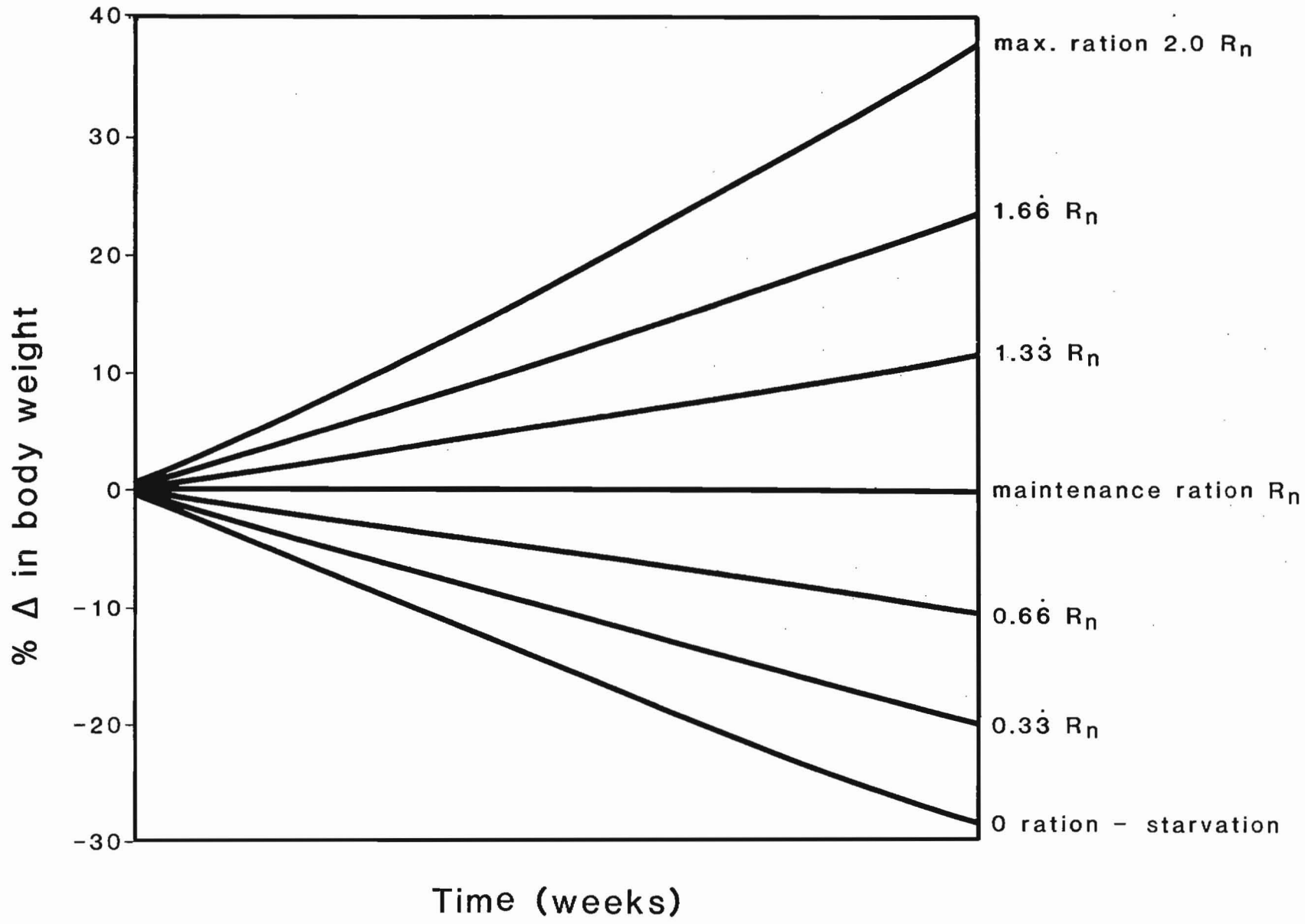


Figure 20. Example of predicted trajectory of average weight over time as a function of percent maintenance ration received.

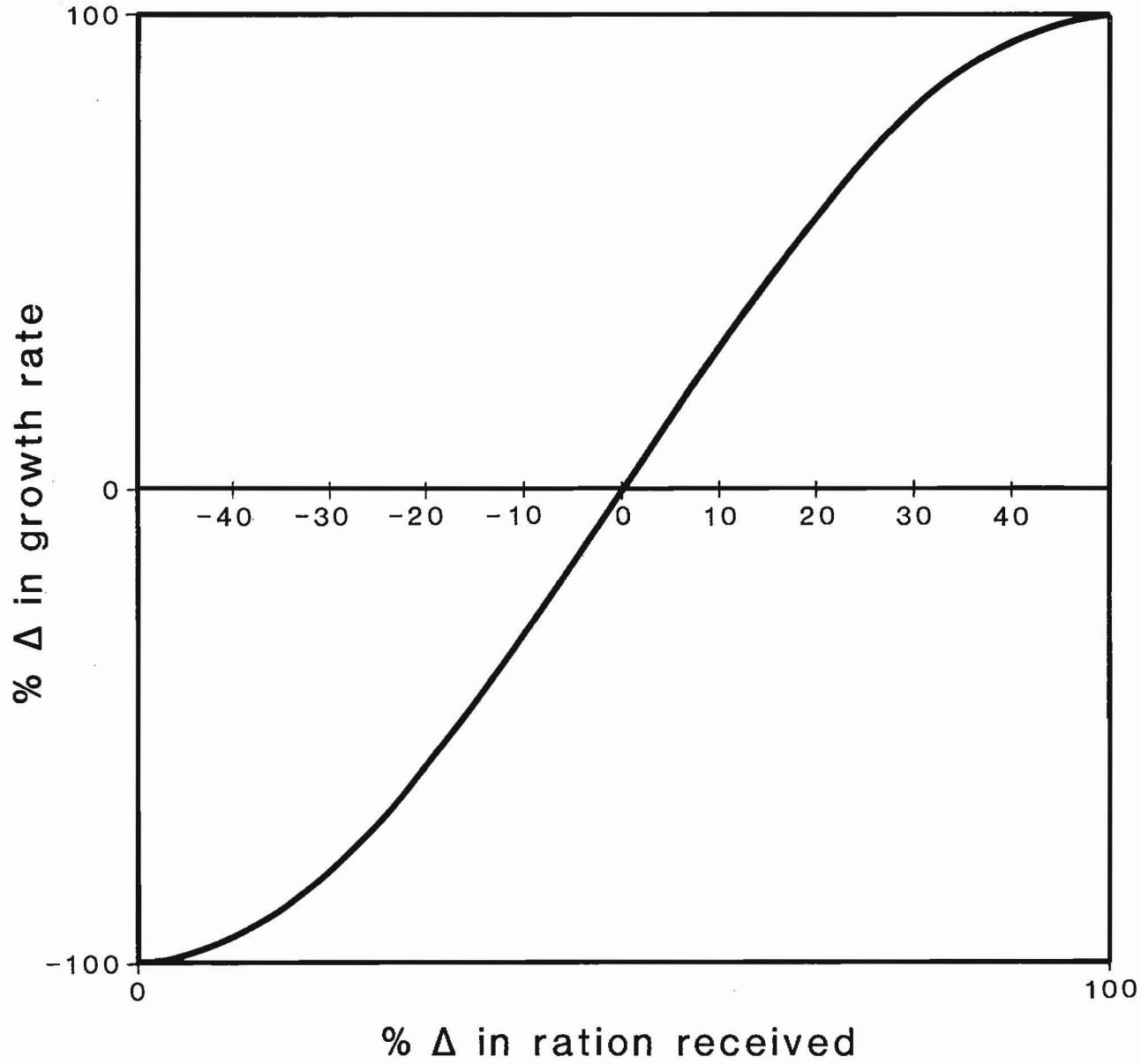


Figure 21. Predicted percentage change in instantaneous growth rate as a function of percentage change in ration received.

Therefore, the discrete approximation becomes:

$$\Delta L = \Delta W * (a * b * L^{b-1})^{-1} \tag{63}$$

Because ΔW can be negative in the model and fish do not decrease in length, the rate of change in length (ΔL) is positive if $\Delta W > 0$ and 0.0 if $\Delta W \leq 0$. Thus:

$$L_{i,t+1} = L_{i,t} + \Delta L \tag{64}$$

where $\Delta L = \Delta W_{i,t} * (a * b * L_{i,t}^{b-1})^{-1}$ if $\Delta W > 0$

and

$= 0.0$ if $\Delta W \leq 0$

The rate of change in length is governed by empirically derived relationships between length and weight and may be quite different from the realized relationship between length and weight in the model. This is because the submodel is constrained to predict no decrease in length if there is a decrease in weight but does predict an increase in length associated with any weight gain following a substantial weight loss. In reality, however, a fish would probably exhibit some initial weight gain without any associated increase in length under these circumstances. Here again, the model provides an interface between traditional fisheries techniques and a systems ecology approach.

As much biological realism as possible has been incorporated in the model. Certainly, a more advanced conceptual approach can, and should be, advocated. However, excessive data requirements on population dynamics and lack of information about indirect effects of pH and aluminum on population dynamics precludes a more sophisticated model at the present time. A better understanding of how fish populations respond to acidification of their environment must be developed if the health of the fishery is to be used as an early indicator of failure of the ecosystem to assimilate acidic inputs.

Chapter Authors: Paul Rago, FWS; and Carl Schofield, Cornell University.

Chapter Contributors (in alphabetical order): L. Barnthouse, Oak Ridge National Laboratory; Peter Daye, Daye Atlantic Salmon Corporation; Ron Eisler, FWS, OBS; Robert Foley, N.Y. Dept. of Environmental Conservation; Eugene Fritz, FWS; Terry Haines, FWS; Dave Lenhart, FWS; Rufus Morrison, Harvard University; Tom Roush, Environmental Research Lab, Duluth; Stan Smith, FWS; and James Weiner, FWS.

8. WATERSHED DATA BASES

Two data bases, one from Harp Lake in Ontario and the other from Filson Creek in Minnesota, were available during the Acid Precipitation Workshops. These data bases were used to parameterize the simulation model and evaluate preliminary model runs.

DATA BASE FROM HARP LAKE, ONTARIO

Data for Harp Lake, supplemented by data in the literature for other lakes, were used in the nominal run of the model. Much of the Harp Lake data is in unpublished form. These data have been used with the permission of W. Scheider and P. J. Dillon (Ontario Ministry of Environment, Rexdale, Ontario), who can be contacted for further information. The data cover the period of October 1977 to September 1978, unless otherwise specified.

Site Description

Harp Lake (45° 23' N, 79° 08' W) is located in Muskoka Township, south-central Ontario, Canada. The bedrock geology of the watershed is composed of gneiss (67%), amphibolite and shist (28%), and diorite (3%). There is a thin (~ 1 m), glacially-derived overburden characterized as minor till plain (50%), thin till and rock ridges (39%), peat and pond (7%), sand (4%), and exposed bedrock (0.3%). The basin is covered with a mixed deciduous-coniferous forest. Although there is no logging activity in the basin at present, the area was logged within the last century. Harp Lake receives an average of 1.0 m of precipitation annually, much of it (~40%) falling as snow between mid-November and early April.

Harp Lake has a total drainage basin area of 575.5 ha, with 508.6 ha of terrestrial drainage and 66.9 ha of lake surface. The lake has six major inflows, which drain 85% of the terrestrial basin. The remaining 15% of the basin drains directly into the lake or is drained by small, intermittent

streams. Further details on the Harp Lake watershed are available from Dillon et al. (1978) and Scheider et al. (1979a).

Hydrology

Precipitation was gauged by a network of eight collectors. Collector location, design, and the method of calculating precipitation was summarized by Scheider et al. (1979a) and Jeffries and Snyder (1981).

Streamflow was gauged at each of the six major basins on a continuous basis, as described by Scheider et al. (1979a, 1979b) and W. Scheider (Ontario Ministry of Environment, Rexdale, Ontario; unpubl. data). Flow for the 15% of the basin that was not gauged was prorated from the gauged portion.

Annual lake evaporation (0.62 m/yr) was assumed equal to that measured in 1978 for Clearwater Lake, near Sudbury, Ontario (Scheider 1982) for purposes of the model. Annual evapotranspiration was set at 40% of annual precipitation (Likens et al. 1977; W. Scheider, Ontario Ministry of Environment, Rexdale, Ontario; unpubl. data).

Precipitation

The input of Na^+, K^+, Ca^{+2}, Mg^{+2}, SO_4^{-2}, Cl^-, NO_3^-, total P, dissolved total P, and total Al from precipitation was measured using a network of eight bulk collectors (Scheider et al. 1979a; Jeffries and Snyder 1981). Dry deposition of SO_2 was estimated using a deposition velocity of 0.6 cm/sec and a $[SO_2]$ of 3.5µg/m³.

Stream Chemistry

Analyses of Ca^{+2}, Mg^{+2}, Na^+, K^+, H^+, SO_4^{-2}, Cl^-, alkalinity (as $CaCO_3$), NO_3^-, NH_4^+, total P, dissolved total P, dissolved organic C, and total Al were done on a weekly basis and combined with streamflow to give a flux value for each of the six streams (Scheider et al. 1979a; W. Scheider and D. Jeffries, Ontario Ministry of Environment, Rexdale, Ontario; unpubl. data). The input

was totaled and prorated to take into account the 15% of the basin that was not gauged. Total flux was divided by the total flow to obtain a mean volume-weighted concentration for each chemical species.

Lake Chemistry

Volume-weighted lakewater samples were collected at the deepest location of the lake (P. Dillon, Ontario Ministry of Environment, Rexdale, Ontario; unpubl. data) at weekly intervals. Samples were analyzed for Ca^{+2}, Mg^{+2}, Na^{+}, K^{+}, H^{+}, SO_4^{-2}, Cl^{-}, alkalinity (as $CaCO_3$), NO_3^{-}, NH_4^{+}, total P, dissolved total P, and Al.

Phytoplankton-Zooplankton

Phytoplankton and zooplankton were sampled through the euphotic zone and the whole lake, respectively, at approximately weekly intervals throughout the open water season. Methods of collection, preservation, identification, and enumeration were summarized by K. Nichols (Ontario Ministry of Environment, Rexdale, Ontario; unpubl. report) and N. Yan (Ontario Ministry of Environment, Rexdale, Ontario; unpubl. report).

Fish

Population estimates of smallmouth bass, creek chub, white sucker, and burbot were available from mark-recapture studies. The age composition of white suckers was obtained for 1979 (H. Harvey, University of Toronto, Toronto; unpubl. data).

DATA BASE FROM FILSON CREEK WATERSHED, MINNESOTA

Site Description

The following site description for the Filson Creek Watershed is from Siegel (1982). Filson Creek and Omaday Lake are in Superior National Forest, 13 km southeast of Ely, Minnesota. Filson Creek watershed above the U.S.

Geological Survey gate covers 25.2 km^2; it contains one major tributary and Omaday and Bogberry Lakes. The watershed is predominantly forested. During the past 75 years, most of the original forest cover of white, jack, and red pine has been cut and replaced by a mixed upland forest of aspen, birch, spruce, and other conifers. About 30% of the watershed is wetland, consisting of fens and black spruce swamp.

Ten to 15% of the watershed is rock outcrop. The remainder is covered by drift and Holocene surficial materials generally less than 1.5 m thick, but as much as 15 m thick in wetland areas.

The mineralogy of the drift reflects the underlying and nearby types of bedrock. Ninety percent of the watershed is underlain by rocks of the Duluth Complex. These rocks are mostly composed of calcic plagioclase, with minor amounts of olivine, orthopyroxene, clinopyroxine, and iron and titanoferric oxides. Generally, the composition of the rock is troctolite, but can vary from anorthosite to gabbro. The northern part of the watershed is underlain by the Giants Range Granite. Most of the granite consists of Microcline, hornblende, and highly altered oligoclase. A mineralized zone that contains both copper and nickel sulfide minerals occurs at the contact between the Giants Range Granite and the Duluth Complex.

Hydrology

Precipitation was gauged at a collector within the watershed in 1979 and within 1 km of the watershed in 1977. Discharge near the mouth of Filson Creek was measured by a continuously recording USGS stream gauge. In addition, six piezometers and interflow collectors were established in the watershed for a rough potentiometric surface and interflow assessment. Moisture content of snow was determined by two snow courses in March, 1976, and three snow courses in March, 1980.

Precipitation

Precipitation samples were analyzed for pH, SO_4^{-2}, and NO_3^- in 1979 and for pH and total SO_4^{-2} in 1977. Bulk snow samples were measured for all major

cations and anions in 1979 by the U.S. Forest Service (G. Glass, U.S. EPA, Duluth, MN; unpubl. data).

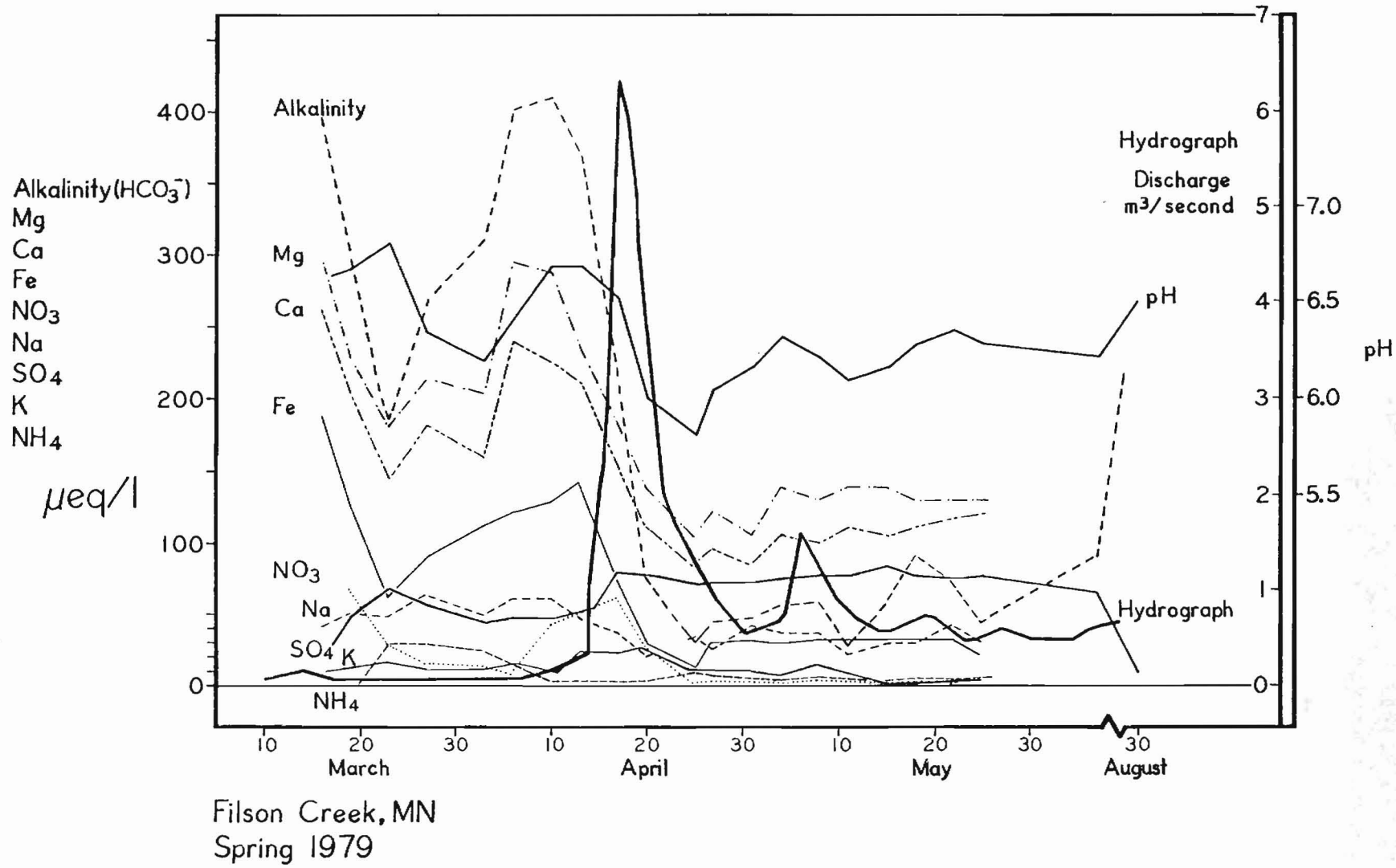
Watershed Chemistry

Water chemistry in the Filson Creek watershed was sampled at six sites, including four tributaries, Omaday Lake outlet, and a downstream creek. In addition, six piezometers and interflow collectors were established in the watershed to determine interflow water quality.

Major anions (NO_3^-, SO_4^{-2}, HCO_3^-, Cl^-, and silica) and cations (Mg^{+2}, Ca^{+2}, Fe^{+2}, Na^+, K^+, and NH_4^+) were determined at biweekly intervals during four study periods: January - July, 1976; January -July, 1977; January - February 1978; and March - June, 1979. The 1979 data set is the most complete and was used as a basis for the modeling effort on Filson Creek (see Fig. 22). Other data sets have been contributed by the U.S. Forest Service and the Minnesota Copper-Nickel study (Minnesota Environmental Quality Board 1979), including the following parameters at all six surface water stations, in bulk snow samples, and in well water samples: turbidity, color, conductivity, pH, alkalinity, acidity, total N, total Kjeldahl nitrogen (TKN), nitrate plus nitrite, chloride, sulfates, hardness, silica, total iron, iron, calcium, magnesium, sodium, potassium, orthophosphate, and chlorophyll-a (with pheophytin correction).

Biological Parameters

Biological information from the Filson Creek area is primarily of a general survey nature, rather than the quantitative measurements of population parameters required for this model. Parameter values used in the model, therefore, represent best estimates or extrapolations from data for other geographical areas.



Filson Creek, MN
Spring 1979

Figure 22. Hydrograph and chemical concentrations for Filson Creek, 1979 (from Glass and Bridges, in press).

9. SIMULATION RESULTS

A simulation model is an abstraction of reality and is, therefore, incomplete. Factors that contribute to the lack of completeness include: (1) the complex systems being modeled are not fully understood; (2) the systems are too complex to model completely even if they were fully understood; and (3) adequate data bases are not available to parameterize the model. Nevertheless, the process of building a model and examining its behavior under a variety of conditions can contribute to understanding the real world system it represents. It can also help in identifying the limitations of the model which affect its usefulness in defining research needs and aiding decisionmakers.

One way to identify the limitations is to input a subset of variables from an actual data set to the model and then compare model output with the values of the other variables in the data set. This simple comparison is one step in the model validation process (Caswell 1976). In this chapter, the present acid precipitation model is compared to the Harp Lake, Ontario and Filson Creek, Minnesota data sets described in Chapter 8. The primary constraint to this type of comparison is the incompleteness of existing data bases. Nevertheless, comparing model behavior with existing data sets helps determine the credibility fo the model, additional data needs, and conceptual gaps in the understanding of system function.

HARP LAKE, ONTARIO

Results from two simulation runs based on the Harp Lake data set are presented below. One-year simulation results are compared to observed data for the period from October 1977 to September 1978; 20-year simulation results are used to explore long term model behavior.

Precipitation data (volume and loadings of chemical constituents) measured at Harp Lake from October 1977 to September 1978 were used as input to the

model. Simulated stream discharge and associated chemical concentrations were compared to actual values for this same time period. Harp Lake has six major inflows but the Harp Lake data were combined to represent a single inflow for purposes of comparison, because the model assumes a single inflow to the lake. The simulated and observed stream hydrographs indicate that the model reproduces the watershed hydrologic budget reasonably well (Fig. 23). Although concentrations of 14 chemical constituents were computed in the model, graphic comparisons of simulated and observed concentrations over a 1-year period for only a few representative constituents are included in this report. Yearly patterns for stream concentrations of total phosphorous, dissolved phosphorous, and ammonium were derived from Harp Lake data and input directly into the model because of the complexity and lack of information on watershed processes affecting these constituents. Simulated values, therefore, match observed values, and comparisons for these constituents are not included.

Regression equations used to calculate stream concentrations of major ionic constituents from streamflow values have squared correlation coefficients (r^2) ranging from < 0.001 to 0.62. This means that stream discharge accounts for only a small portion of the variability in streamflow concentrations of most ions. Simulated concentrations match actual average annual concentrations fairly well but only partially capture seasonal dynamics. This fact is illustrated in Figures 24-27, which include simulated and actual concentrations of two of the major cations (Ca^{+2} and Na^{+}) and two of the major anions (SO_4^{-2} and NO_3^{-}). The resulting electroneutrality balance yielded the yearly stream pH pattern in Figure 28. In general, simulated pH is about 1 unit higher than observed. One contributing factor to this difference is that the system, as modeled, is poorly buffered around a pH level of 6. Therefore, the simplified electroneutrality balance equation in the Water Chemistry Submodel is very sensitive to changes in constituents included in the calculation. The omission of seemingly minor constituents from this equation or small errors in terms included in this equation can result in relatively large differences in simulated pH levels. The spring pH depression in the model is due to an increase in anions and decrease in cations during that period (Figs. 24-26). The fact that this depression in the model is less than observed is in large part due to the failure of the streamflow-NO_3 regression to reproduce the actual spring pulse of NO_3 (Fig. 27). The fall pH depression (Fig. 28) is due primarily to

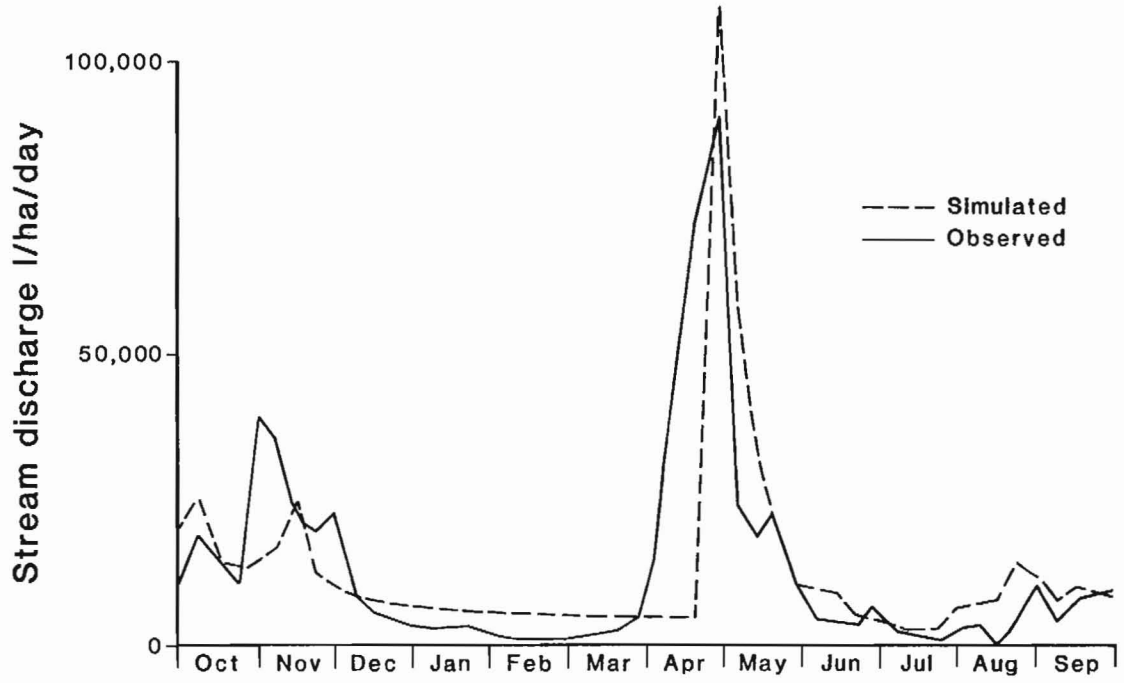


Figure 23. Simulated and observed stream discharge--Harp Lake (1-year model run).

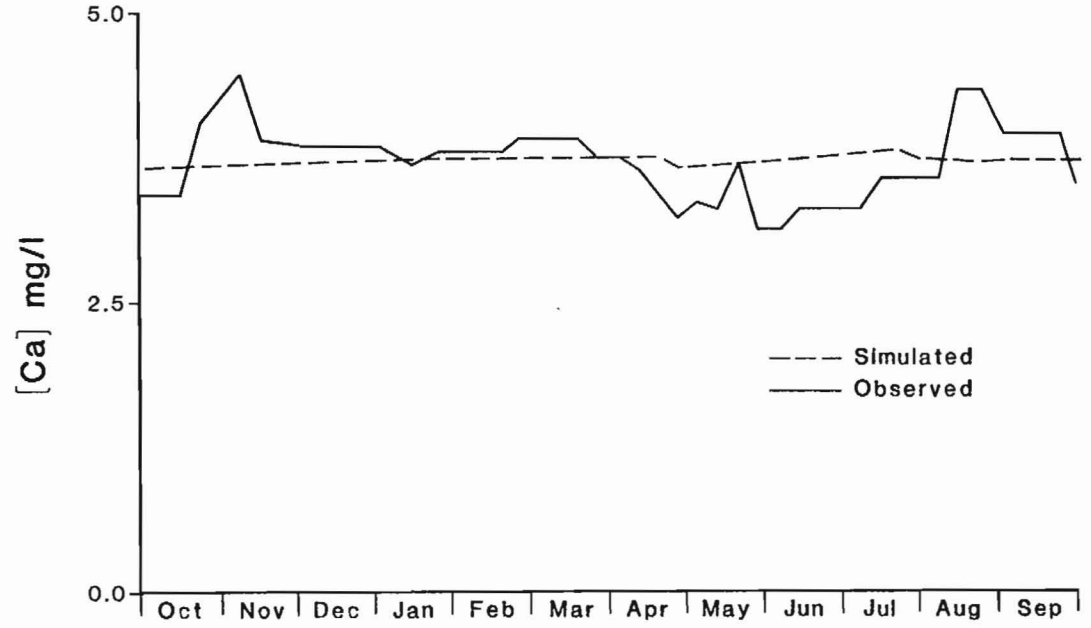


Figure 24. Simulated and observed stream [Ca]--Harp Lake (1-year model run).

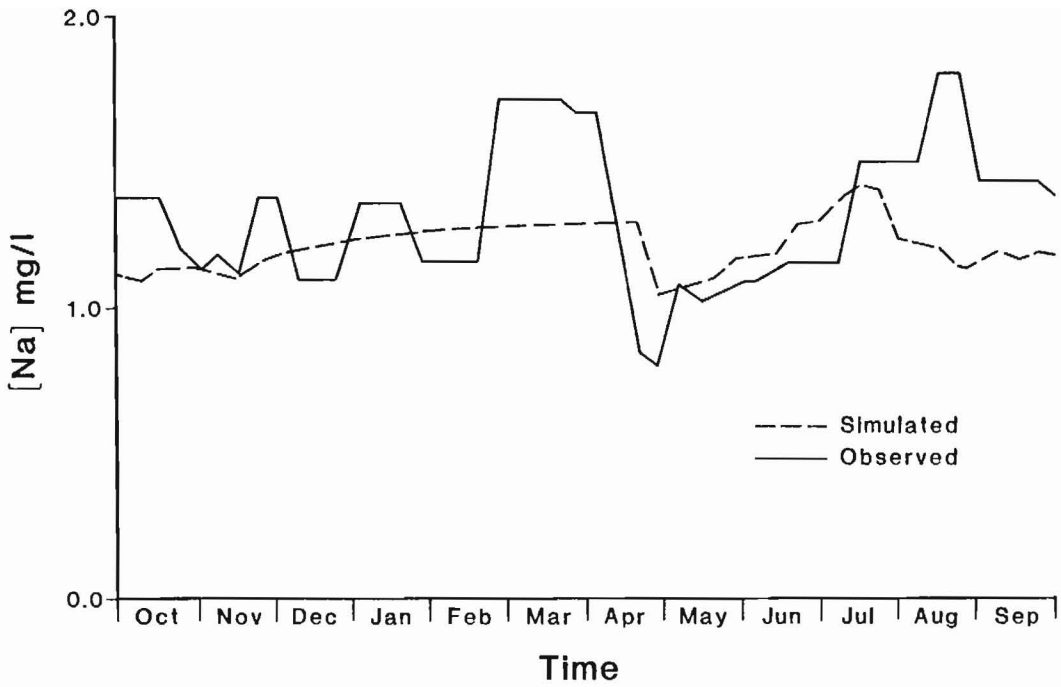


Figure 25. Simulated and observed stream [Na]--Harp Lake (1-year model run).

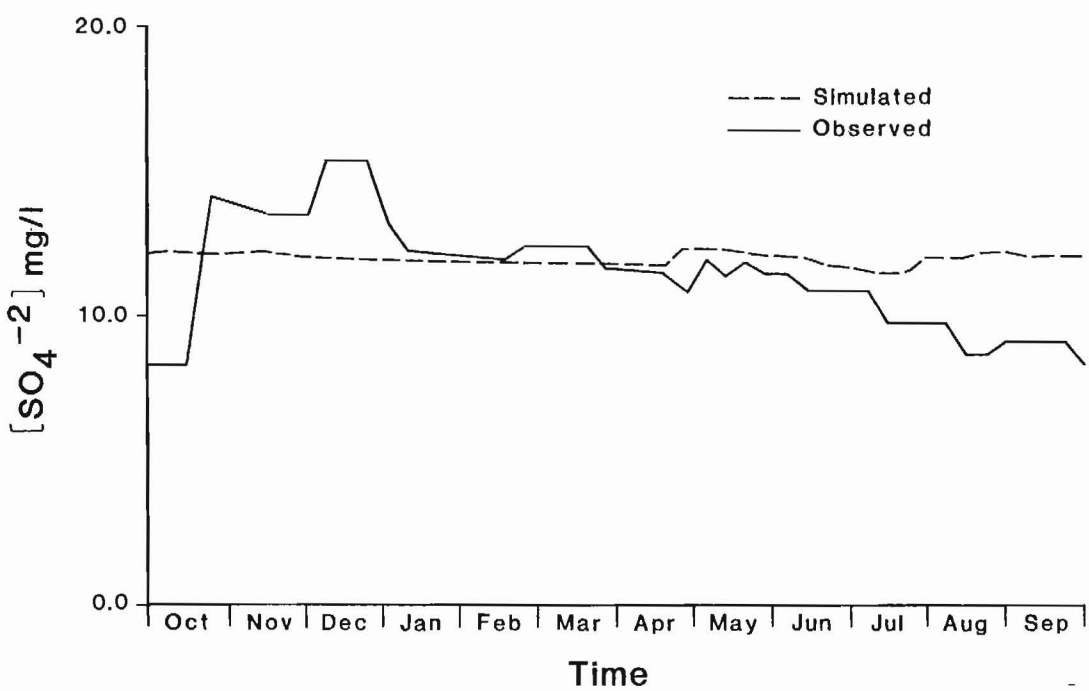


Figure 26. Simulated and observed stream [SO_4-S]--Harp Lake (1-year model run).

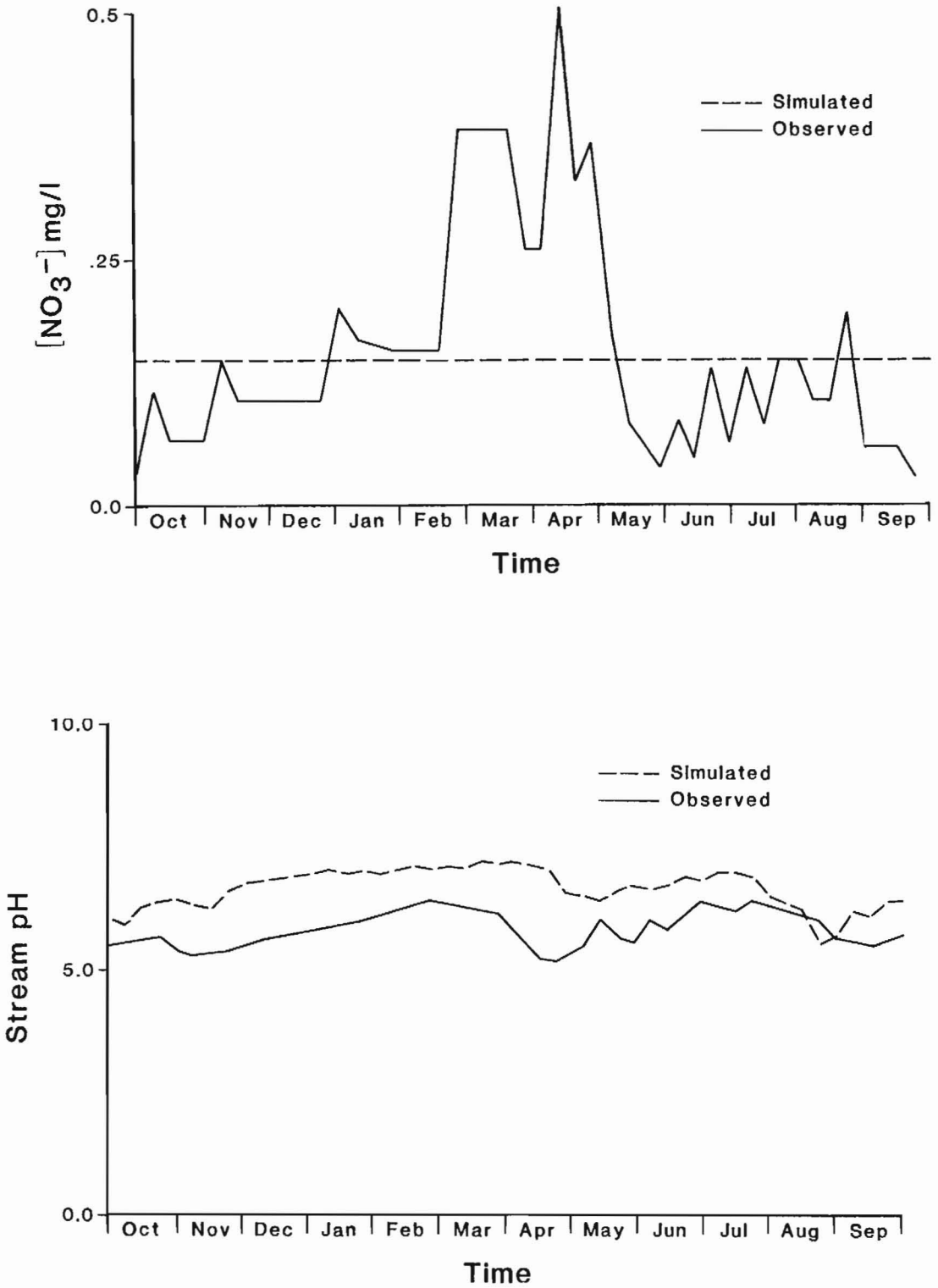


Figure 28. Simulated and observed stream pH--Harp Lake (1-year model run).

the large increase in DOC at that time (Fig. 29). The overestimate of fall and winter pH is caused by an underestimate of the major anionic constituents SO_4 (Fig. 26) and DOC (Fig. 29).

Comparisons of simulated and observed concentrations of major cation constituents in Harp Lake show patterns similar to those for the stream (as illustrated in Fig. 30 for Na^+); that is, reasonable approximation of average annual concentrations but not of seasonal dynamics. Simulated anion constituents show a similar lack of seasonal dynamics, with simulated values slightly higher than observed values (as illustrated in Fig. 31 for SO_4^{-2}). As a result, comparison of simulated and observed lake pH shows a pattern similar to stream pH but with somewhat less discrepancy (Fig. 32).

The Plankton-Benthos Submodel is driven largely by the input and cycling of phosphorous. Despite the complexity of this cycling process, simulated concentrations of available phosphorous agree reasonably well with observed concentrations in Harp Lake (Fig. 33). Observed data for algal chlorophyll and zooplankton were obtained sporadically throughout the year and are not compared to simulated values (Fig. 34). However, simulated values are within the bounds of the available data and exhibit peaks at the proper time of the year. No data are available from Harp Lake on benthos; simulation results are presented in Figure 35. Simulated fish populations exhibit little seasonal dynamics, and results are presented only for the 20-year model run described below.

Stream discharge is computed for any year in the 20-year simulation run from input precipitation data modified by a small random component of year to year variation. As a result, stream concentrations of major ionic constituents and associated stream pH exhibit very little year to year variation (as illustrated in Fig. 36 for pH). Lake concentrations and pH, however, do change over the 20-year simulation run. Cations tend to increase slightly in concentration (Fig. 37), while concentrations of major anion constituents increase more dramatically (Figs. 38-40). As a result, the lake acidifies from an initial pH of 7.2 to a final pH of 5.5 (Fig. 41). The decrease in lake pH results in an initial decrease in inorganic aluminum concentration with, a subsequent increase as pH continues to decline (Fig. 42). Inorganic aluminum

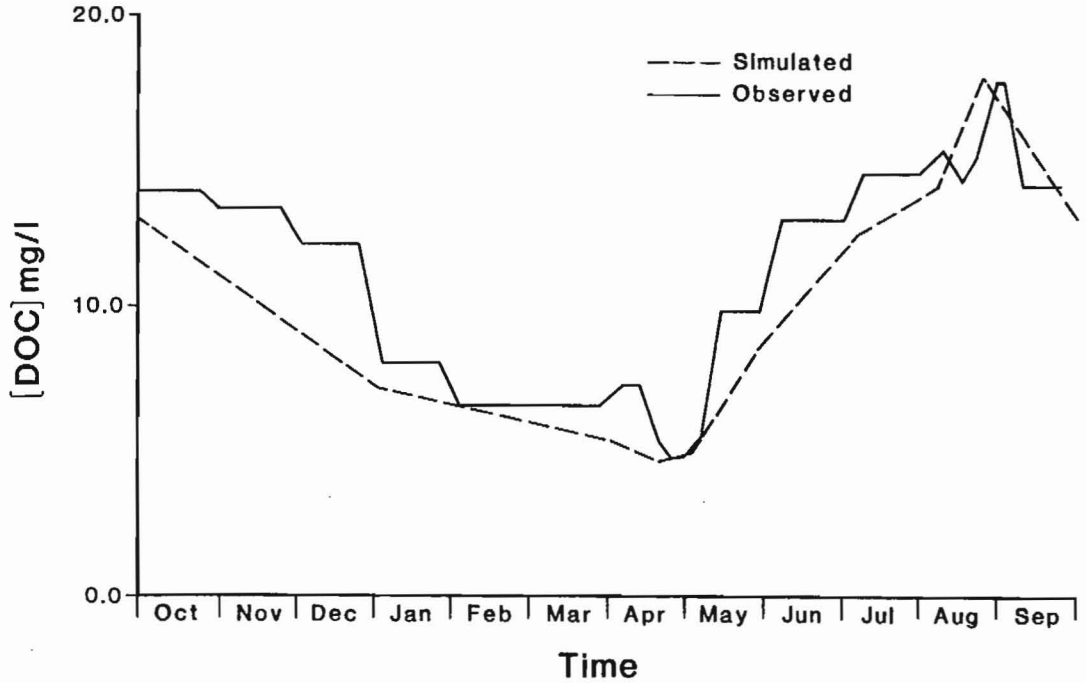


Figure 29. Simulated and observed stream [DOC]--Harp Lake (1-year model run).

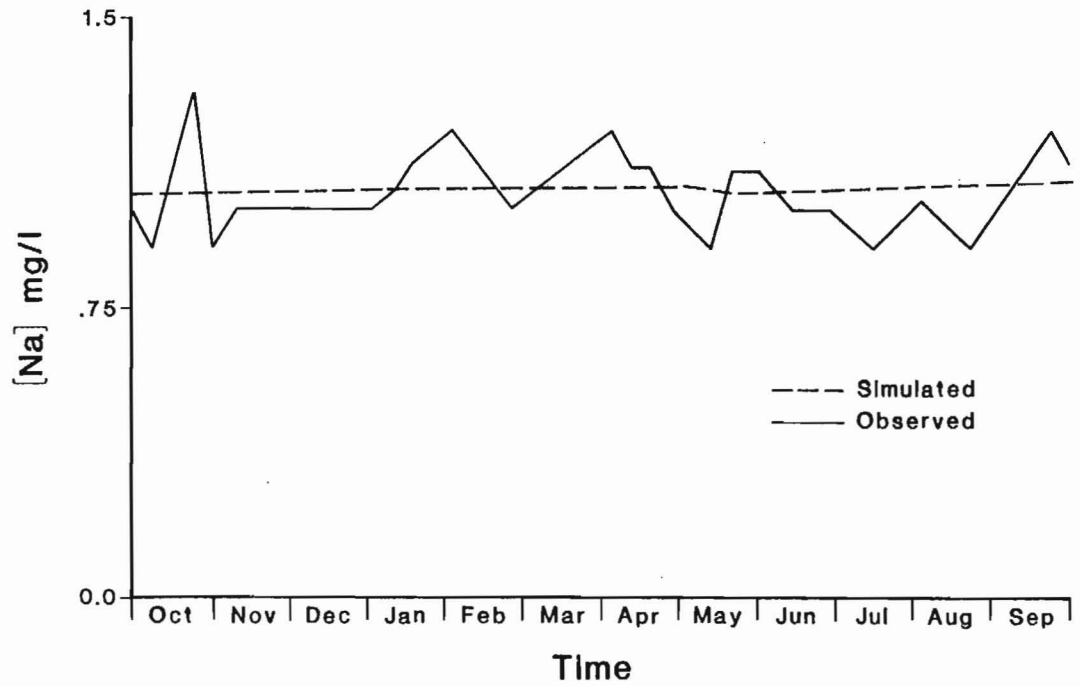


Figure 30. Simulated and observed lake [Na]--Harp Lake (1-year model run).

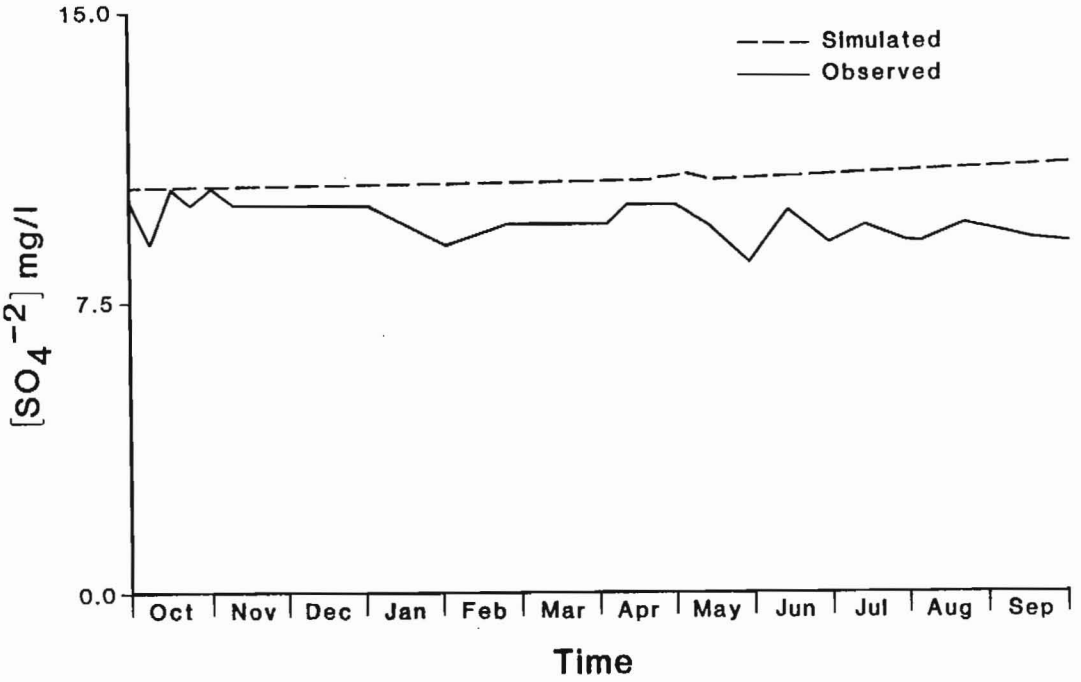


Figure 31. Simulated and observed lake [SO_4-S]--Harp Lake (1-year model run).

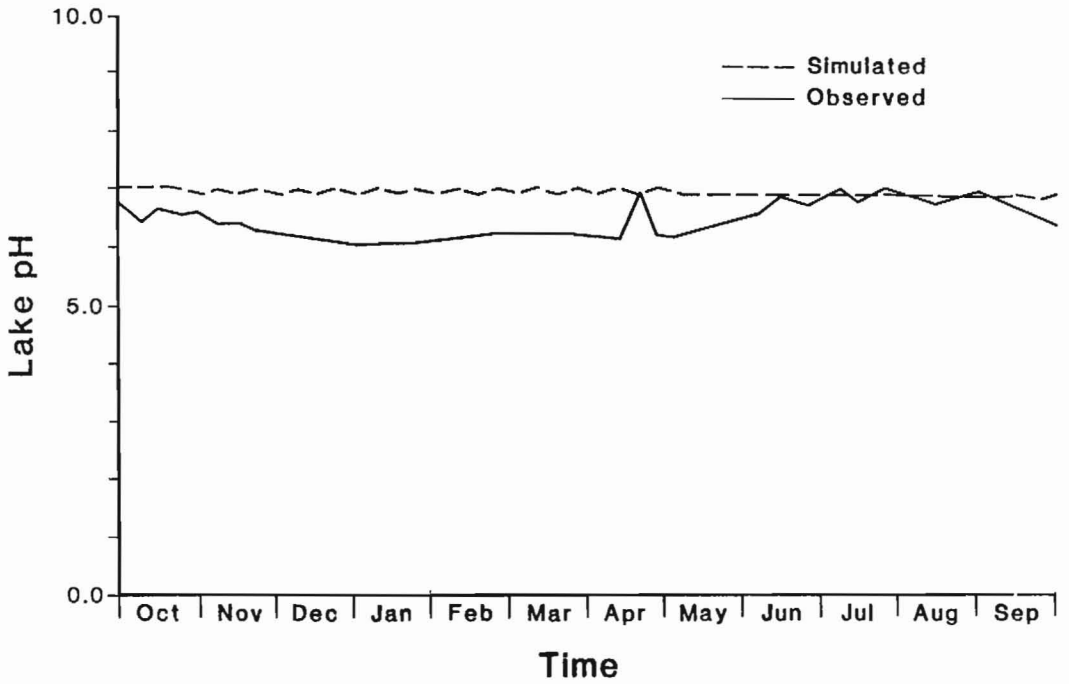


Figure 32. Simulated and observed lake pH--Harp Lake (1-year model run).

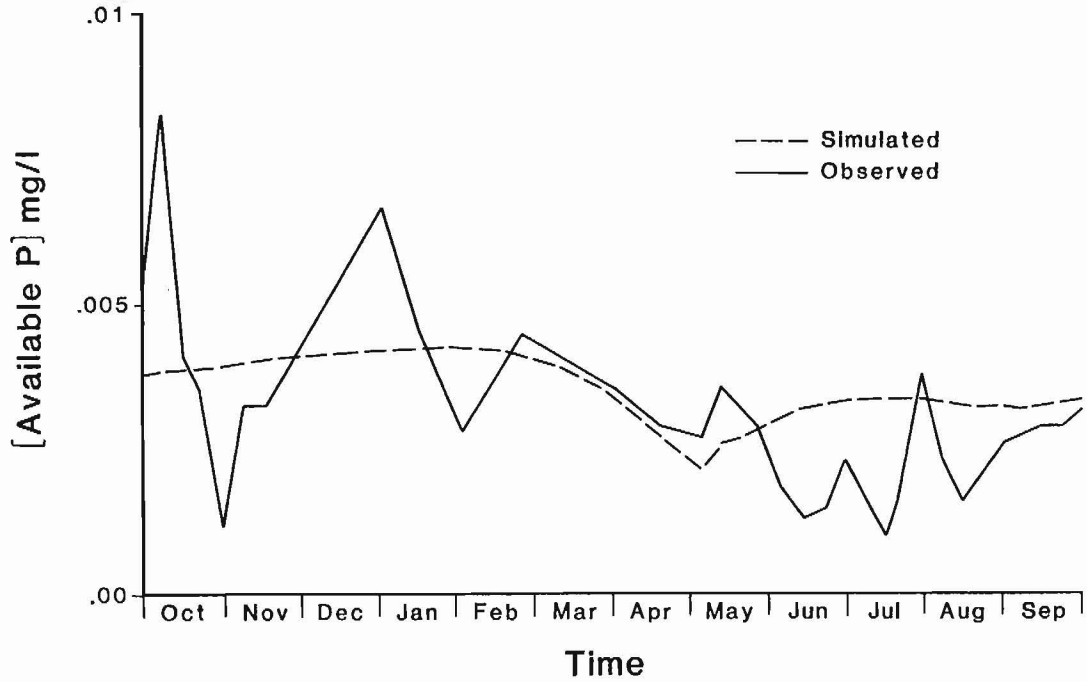


Figure 33. Simulated and observed [available P]--Harp Lake (1-year model run)

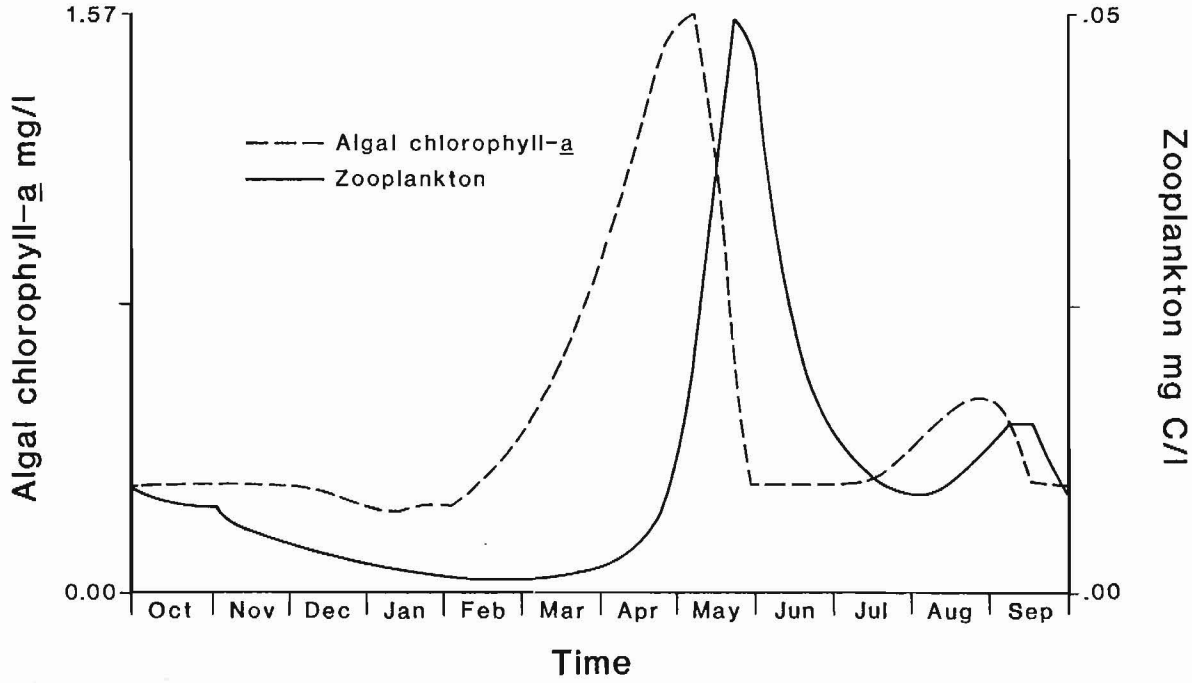


Figure 34. Simulated algal chlorophyll-a and zooplankton C--Harp Lake (1-year model run).

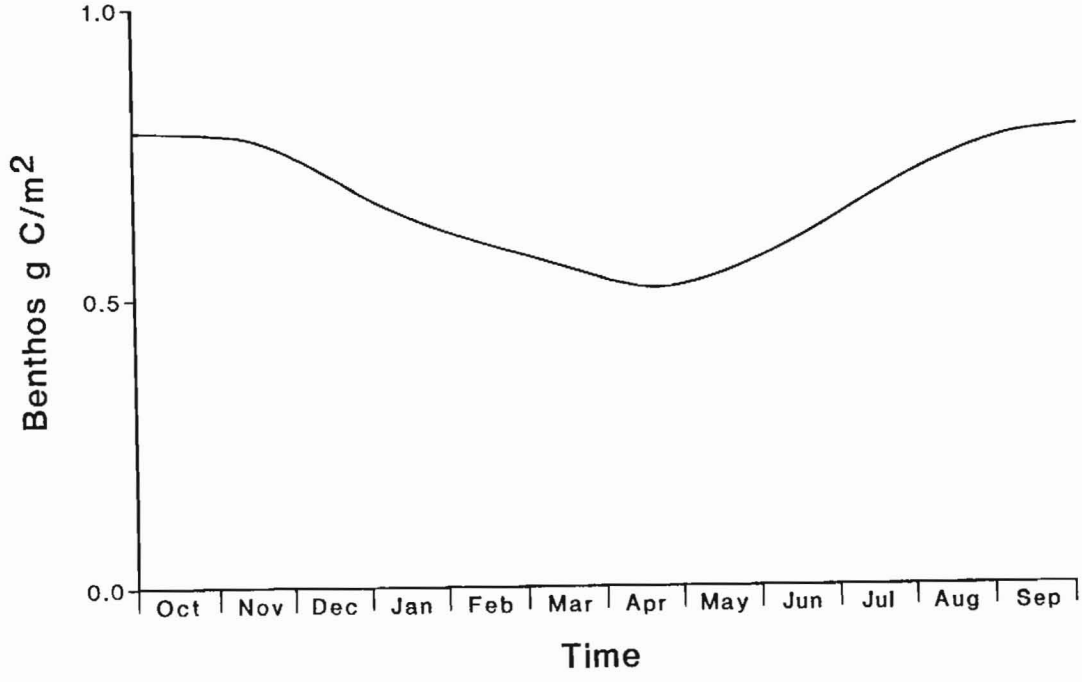


Figure 35. Simulated benthos C--Harp Lake (1-year model run).

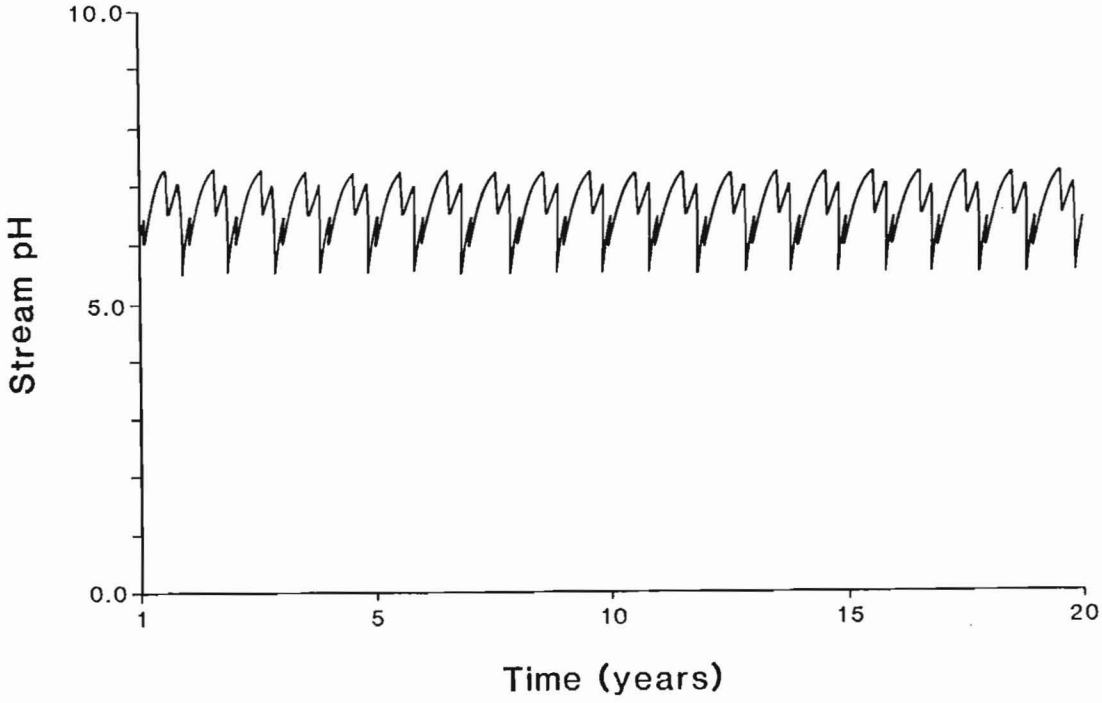


Figure 36. Simulated stream pH--Harp Lake (20-year model run).

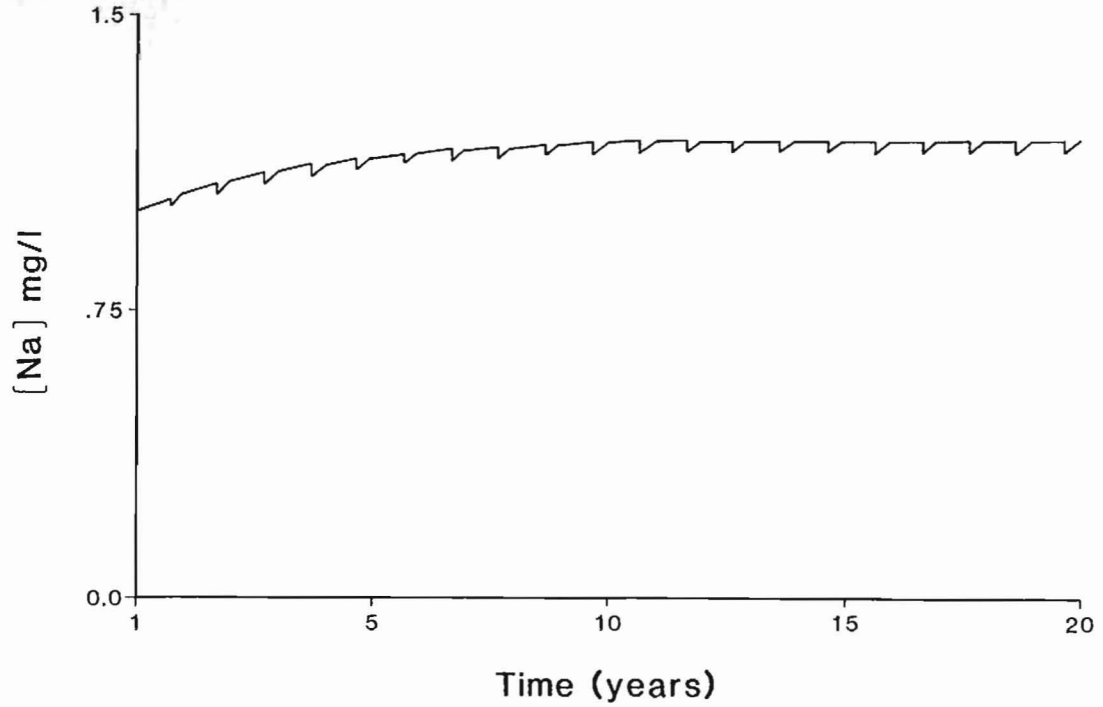


Figure 37. Simulated lake [Na]--Harp Lake (20-year model run).

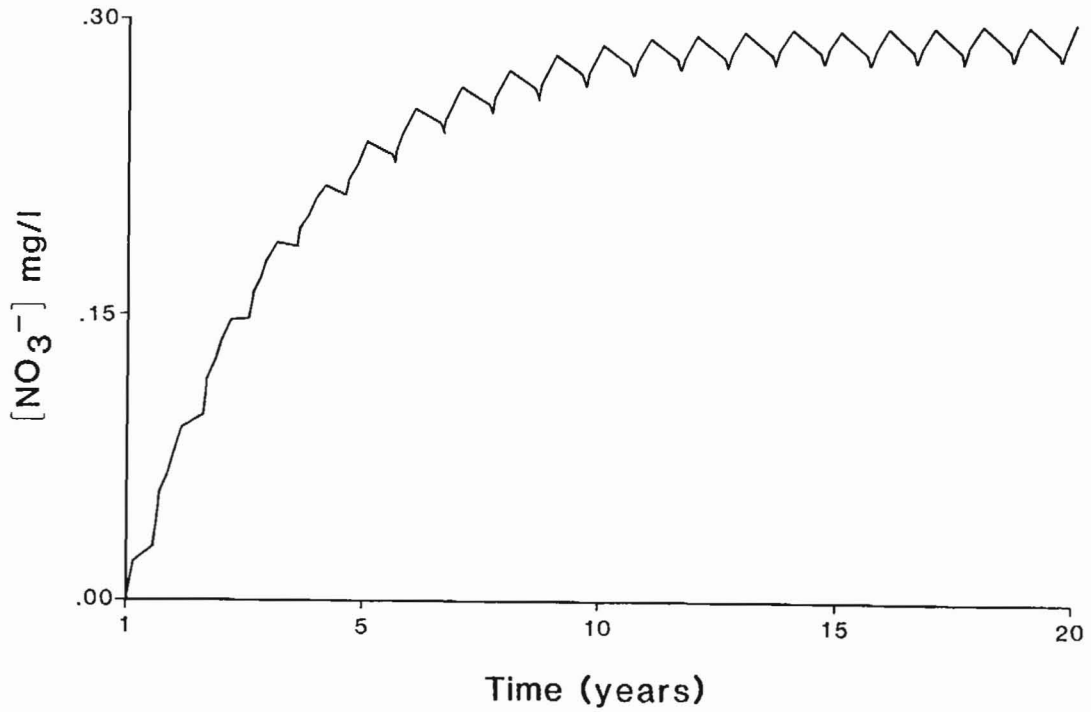


Figure 38. Simulated lake [NO_3-N]--Harp Lake (20-year model run).

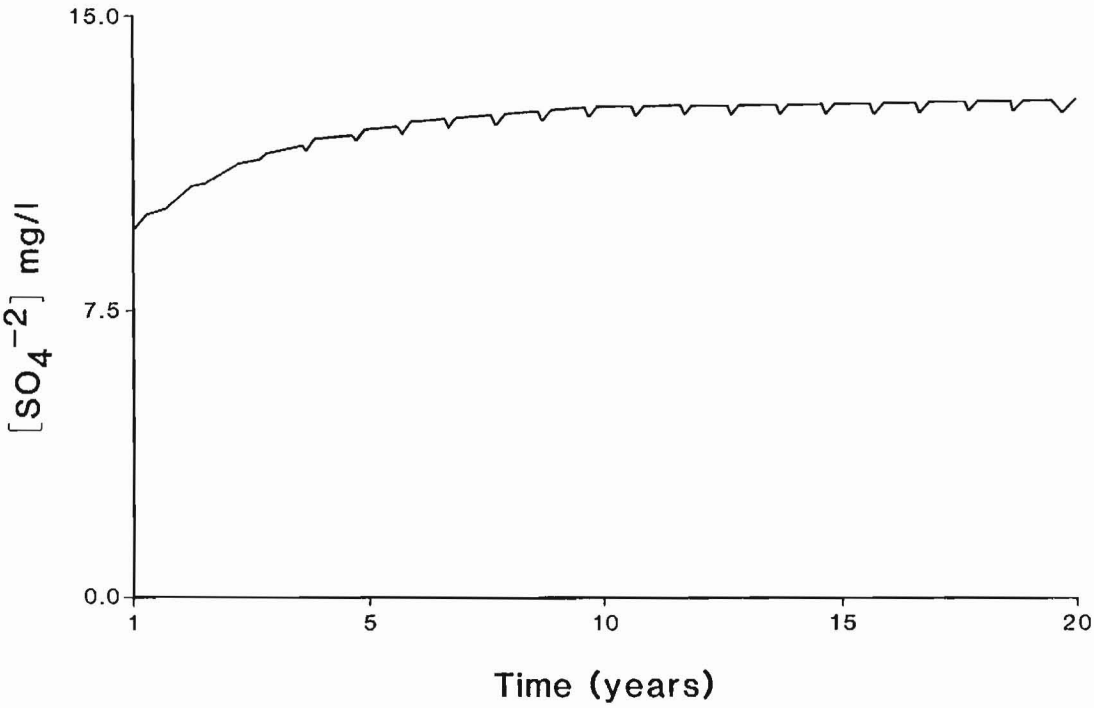


Figure 39. Simulated lake [SO_4-S]--Harp Lake (20-year model run).

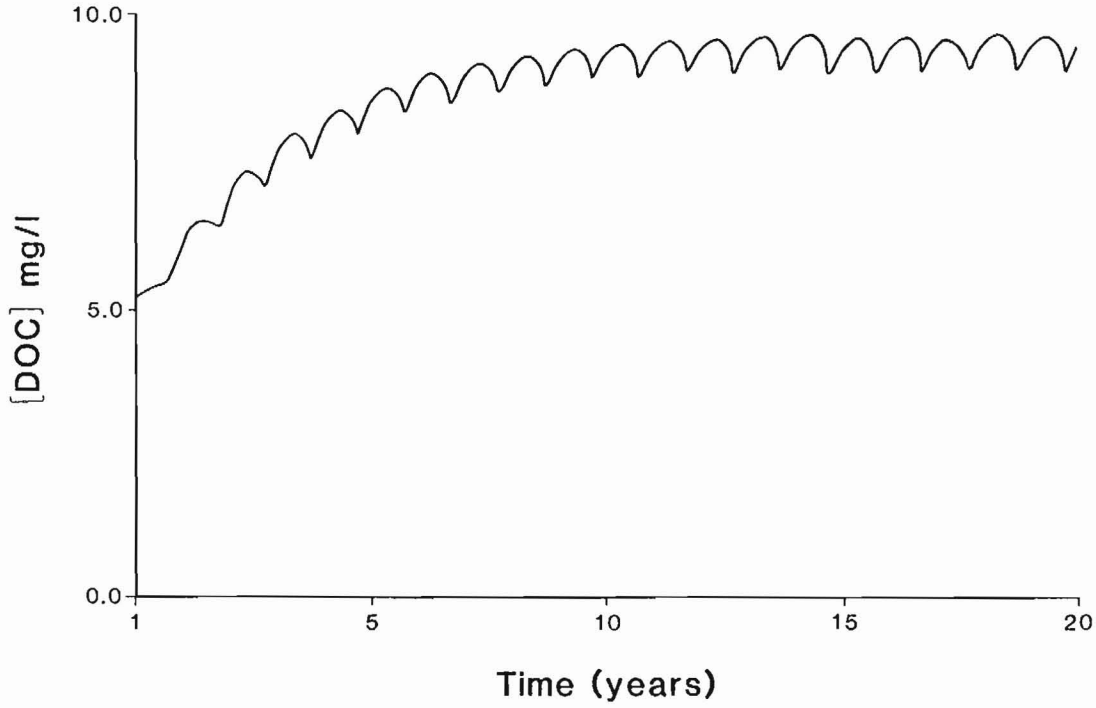


Figure 40. Simulated lake [DOC]--Harp Lake (20-year model run).

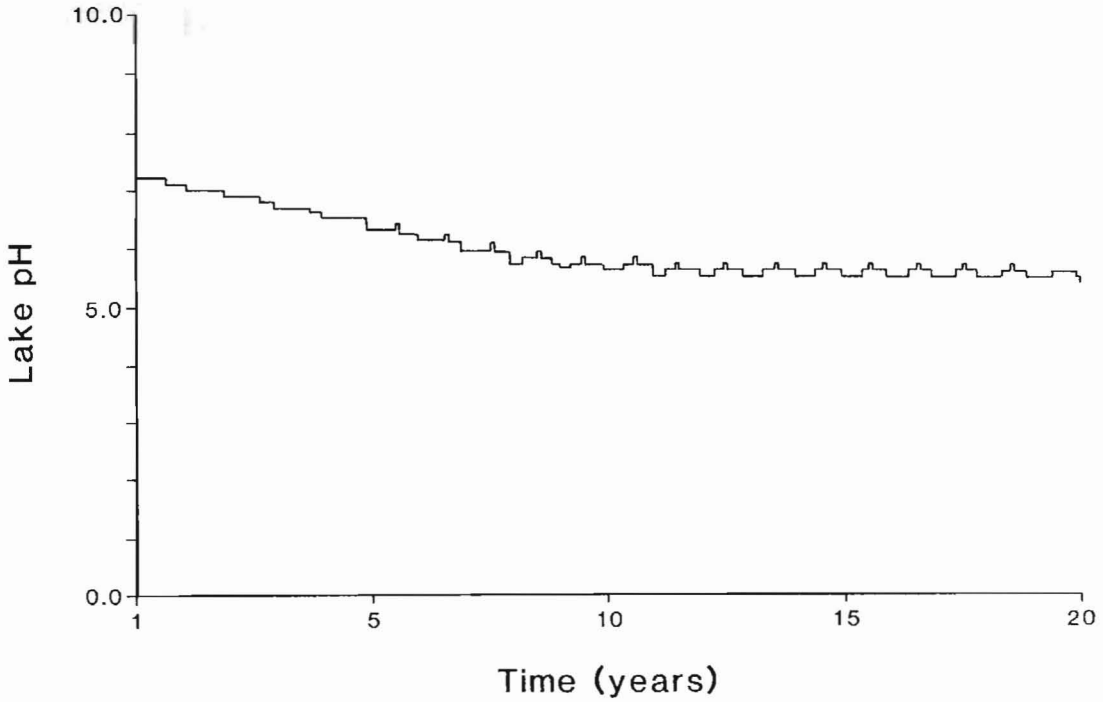


Figure 41. Simulated lake pH--Harp Lake (20-year model run).

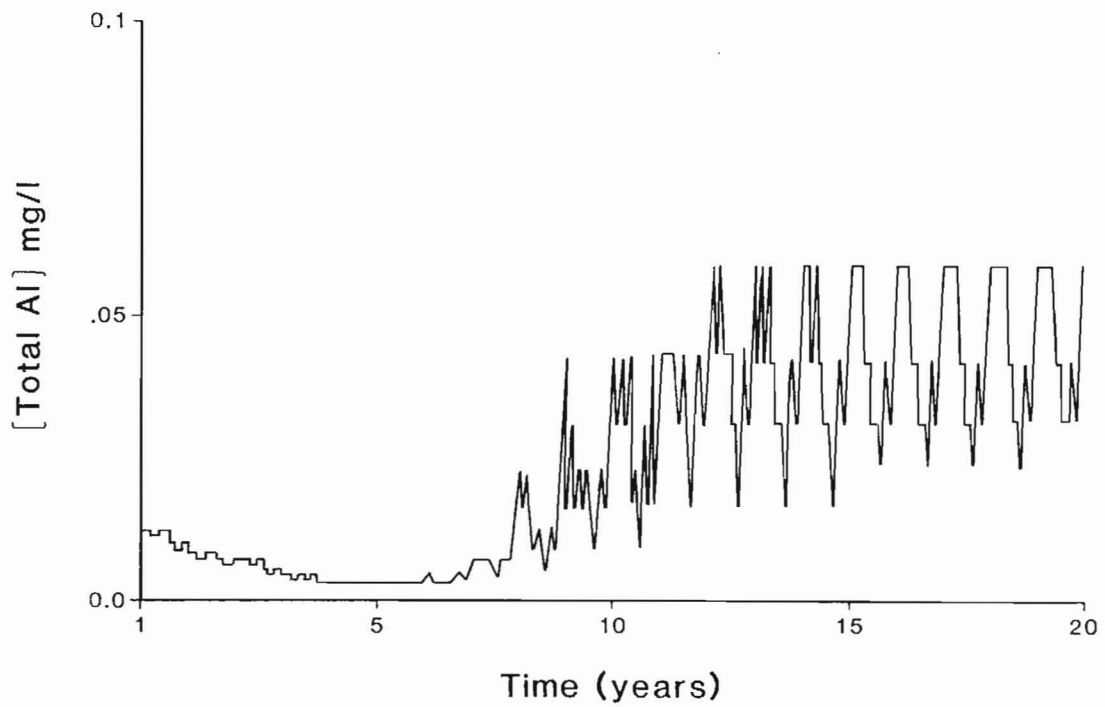


Figure 42. Simulated lake [total Al]--Harp Lake (20-year model run).

is formulated as the sum of seven dissolved aluminum species. Concentrations of these species are formulated as various power functions of $[H^+]$, some of which are directly related to $[H^+]$ and some inversely related. Thus, the relative proportions of the various species change as pH changes, resulting in the decreasing, then increasing, inorganic aluminum concentrations in Figure 42.

The decrease in lake pH has no direct effect on algae, zooplankton, or benthos in the model because it never falls below 5.5. Simulated brook trout populations also show no effects from the pH-aluminum changes. The more sensitive white suckers, however, exhibit a decline in population numbers as a result of lake acidification and the increase in inorganic aluminum (Fig. 43). This decline is caused by increased mortality at the time of hatching. In Figure 43, the decreasing annual increment in population size after year 6 reflects the recruitment of decreasing numbers of young of the year into the adult population.

FILSON CREEK, MINNESOTA

Precipitation data used as input for the simulation of the Filson Creek watershed came from two sampling stations from October 1978 to September 1979. Precipitation volume was measured at the Winton Power Station approximately 19 km from the watershed. The closest chemical constituent data were from Marcell, approximately 160 km west of Filson Creek. Only limited watershed data were available for comparison with simulation results. Stream discharge information for October 1978 to September 1979 from a gauging station below approximately 60% of the watershed was used to evaluate the simulated stream hydrograph. Chemical concentration data for the stream consisted of only 18 samples from March to May 1979. Biological information from the Filson Creek area was primarily of a survey nature and of limited value in evaluating simulation results. Because only limited data were available for Filson Creek, model results are presented primarily to demonstrate general model behavior rather than as part of a quantitative validation process. For any year in a multiple-year simulation run, stream discharge is computed from input precipitation data modified by a small random component of year to year

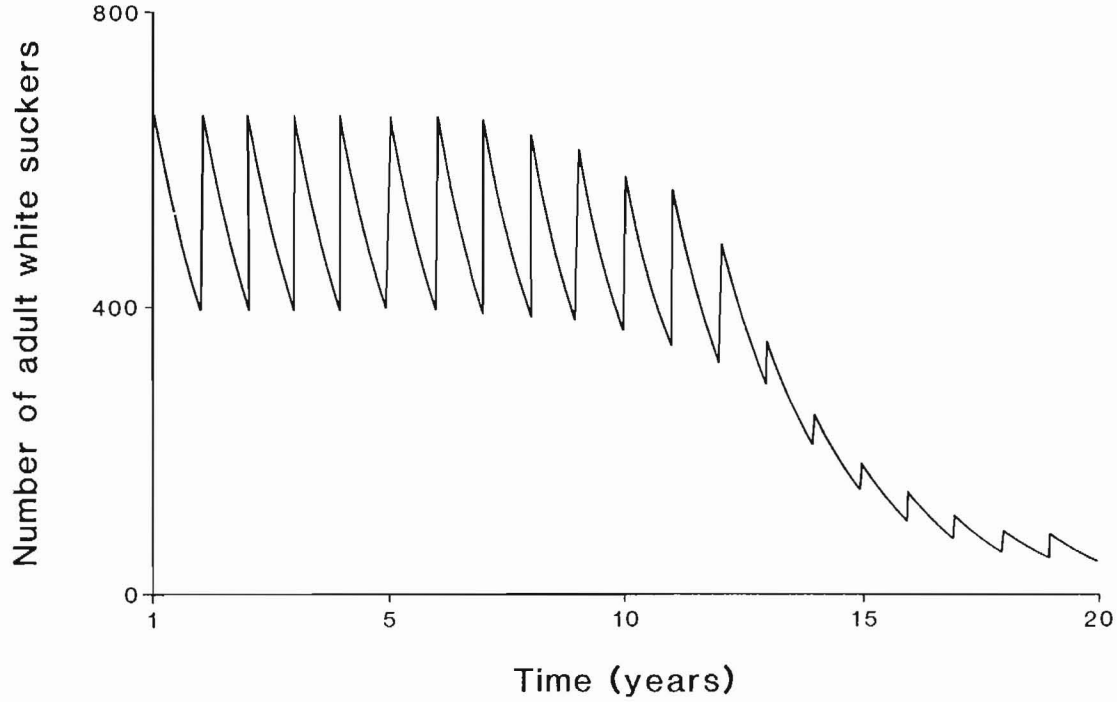


Figure 43. Simulated number of adult white suckers--Harp Lake (20-year model run).

variation. As a result, stream concentrations of major ionic constituents and associated stream pH exhibit very little year to year variation. Therefore, results from a 20-year simulation run are not presented for Filson Creek.

Streamflow simulations did not initially match observed data very well. The problem was a difference between surficial geology of the Filson Creek area and Watershed Submodel assumptions (D. Siegel, U.S. Geological Survey, St. Paul, MN; personal communication). The soil system around Filson Creek is a rapid, shallow, flow-through system where water has minimal contact time; however, 30% of the watershed is wetlands which provide significant surface water storage. Previous attempts to model Filson Creek streamflow which did not include reservoir routing techniques to account for this storage failed miserably. The original Watershed Submodel assumed that all snowmelt moved as quickflow; that is, none of the snowmelt percolated to the lower soil layer to be stored as soil moisture. For Filson Creek model runs, the Watershed Submodel was changed so that the rational equation (1) applied to snowmelt, as well as precipitation, thus allowing storage of some snowmelt in the lower soil layer. While this storage represents a different physical process than wetland surface storage, it provides a surrogate reservoir routing mechanism and the resulting simulated stream hydrograph matches the observed hydrograph reasonably well (Fig. 44).

Because chemical concentration data for Filson Creek were only available for a 3-month period during the spring, the usefulness of the resulting regression equations (r^2 ranging from 0.01 to 0.88) in predicting concentrations throughout the year is unknown. Simulated and observed concentrations of Ca^{+2} and SO_4^{-2} are presented in Figures 45 and 46, respectively. Other major ionic constituents compare to observed data in a similar way. An electroneutrality balance of ionic constituents results in the stream pH pattern in Figure 47. Simulated pH is about 1 unit higher than observed spring data. In addition to the sensitivity of the electroneutrality equation discussed earlier, D. Siegel (U.S. Geological Survey, St. Paul, MN; personal communication) offers a possible explanation for this discrepancy. The Water Chemistry Submodel assumes that the various dissolved aluminum species are in equilibrium with an $Al(OH)_3$ mineral phase but the submodel does not consider chelation reactions such as complexation of organic acids and aluminum. Siegel notes that

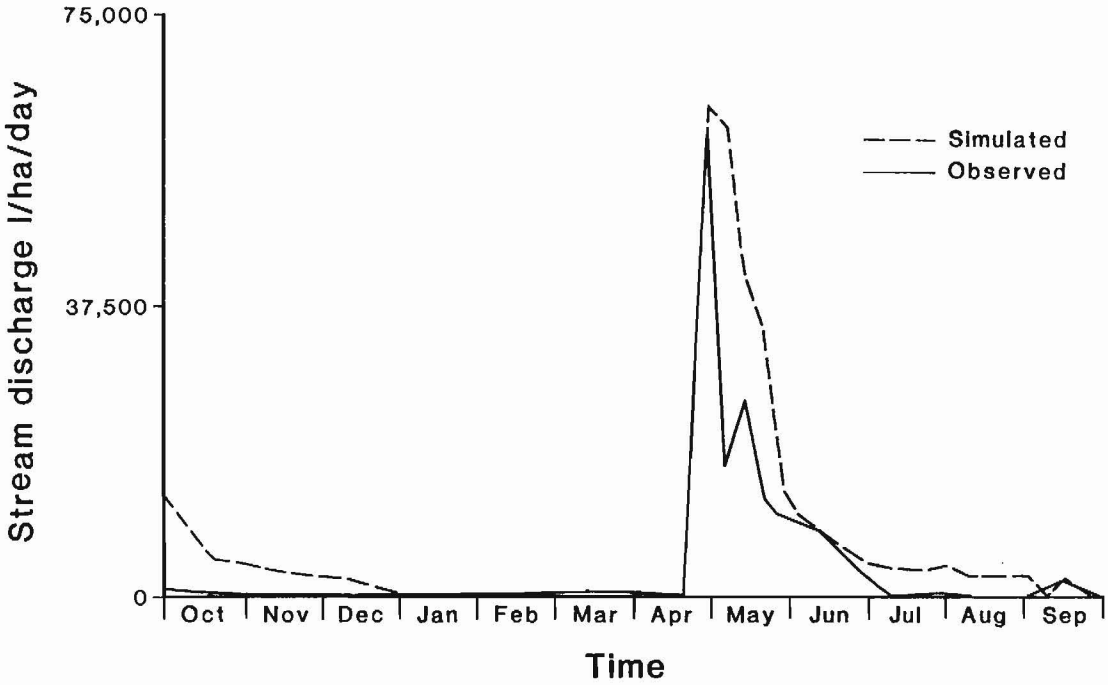


Figure 44. Simulated and observed stream discharge--Filson Creek (1-year model run).

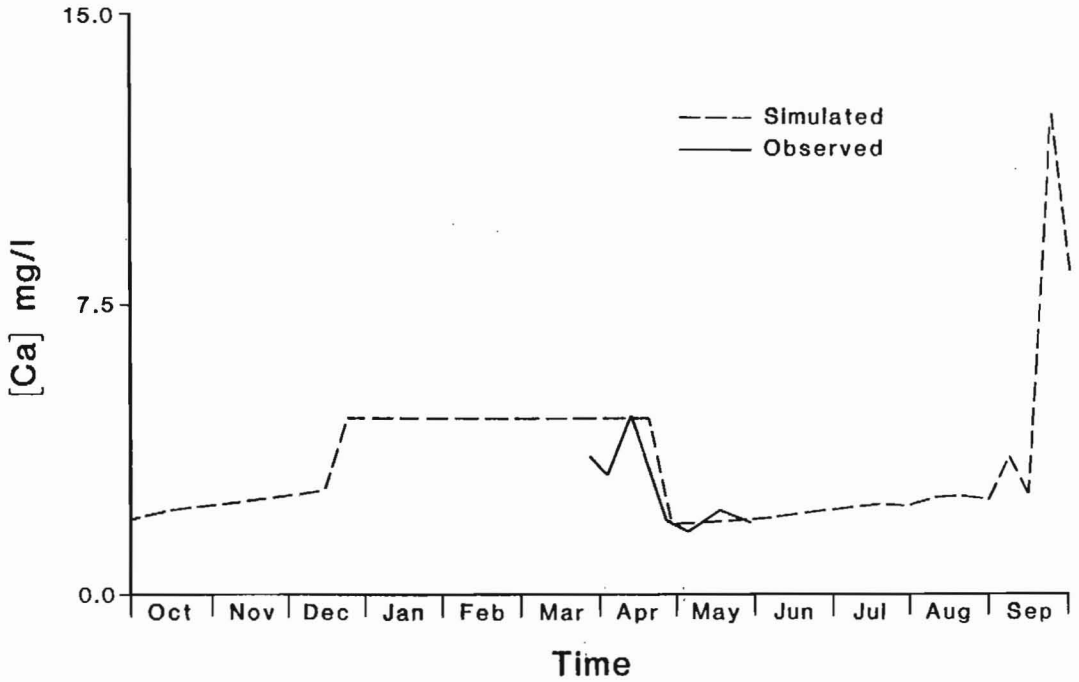


Figure 45. Simulated and observed stream [Ca]--Filson Creek (1-year model run.

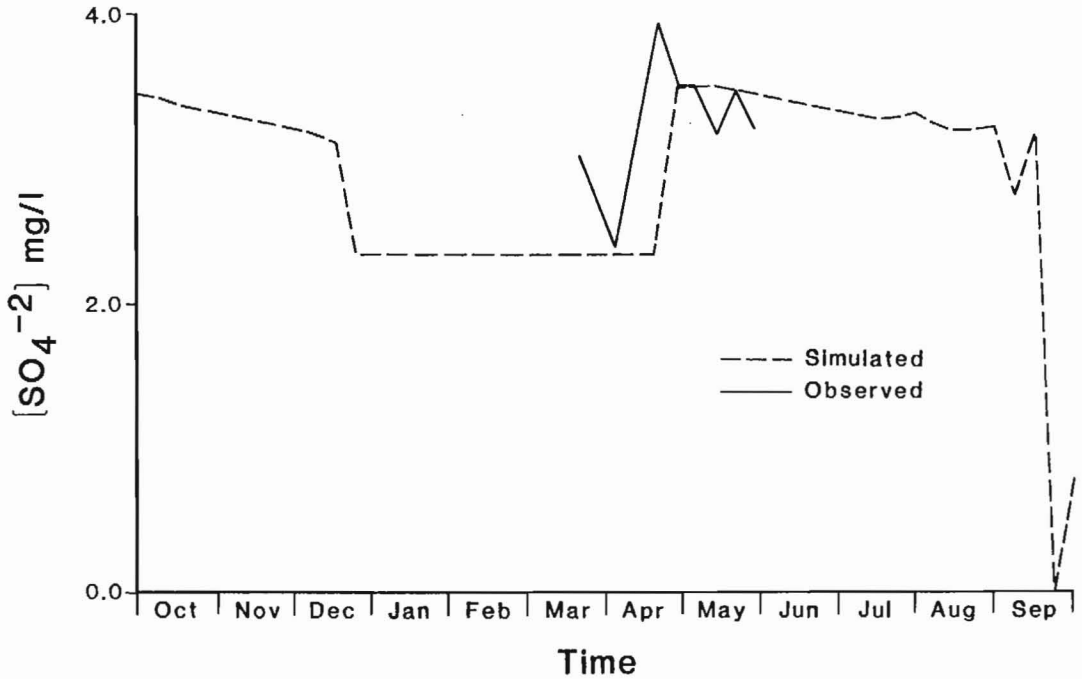


Figure 46. Simulated and observed stream [SO_4-S]--Filson Creek (1-year model run).

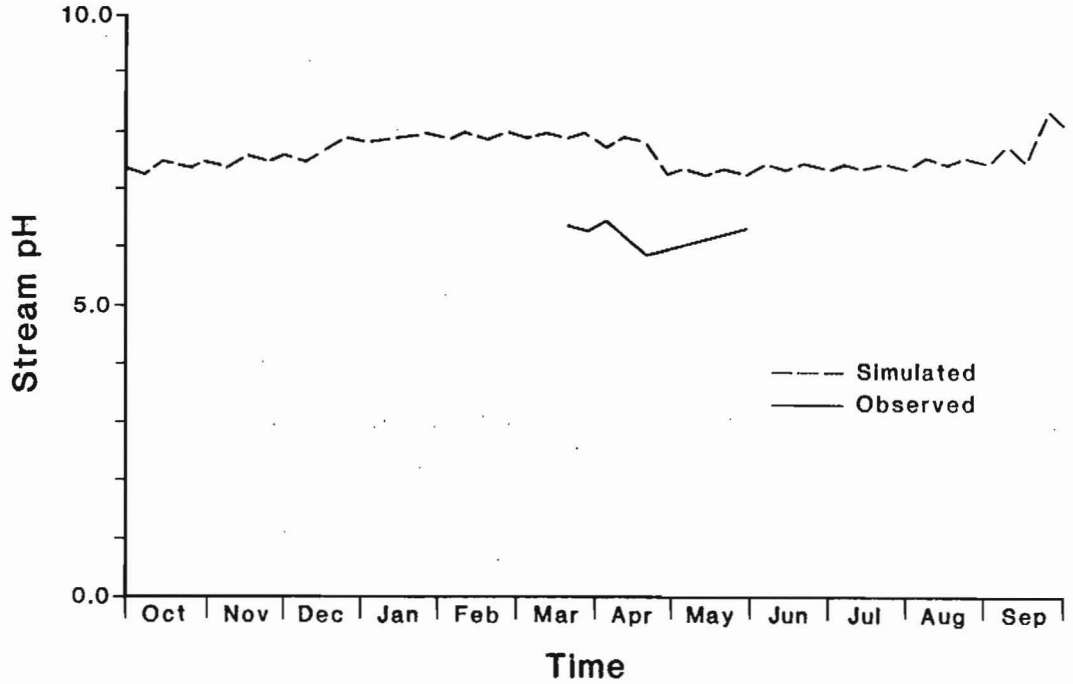


Figure 47. Simulated and observed stream pH--Filson Creek (1-year model run.

crystalline gibbsite [$Al(OH)_3$] has not been found in sediments at Filson Creek. In addition, the high observed concentrations of DOC (up to 30 mg/l) and aluminum (200-300 µg/l) suggest Al complexation by organic acids. Simulated DOC and total aluminum are presented in Figures 48 and 49, respectively.

The Plankton-Benthos Submodel is driven primarily by inputs of allochthonous material and light. Seasonal data for these inputs are not available. In addition, biological information from the Filson Creek area is primarily of a general survey nature. Because of this lack of quantitative data, simulated levels of periphyton and grazers (Fig. 50), shredders and collectors (Fig. 51), and fish (Fig. 52) are included only to demonstrate general model behavior. Figure 52 reflects observations that Filson Creek is used by white suckers for spawning in the spring but does not support a resident population. An intermittent, cool water stream, such as Filson Creek, would support some resident fish populations (e.g., various Cyprinid species); however, the Fish Submodel does not include these species.

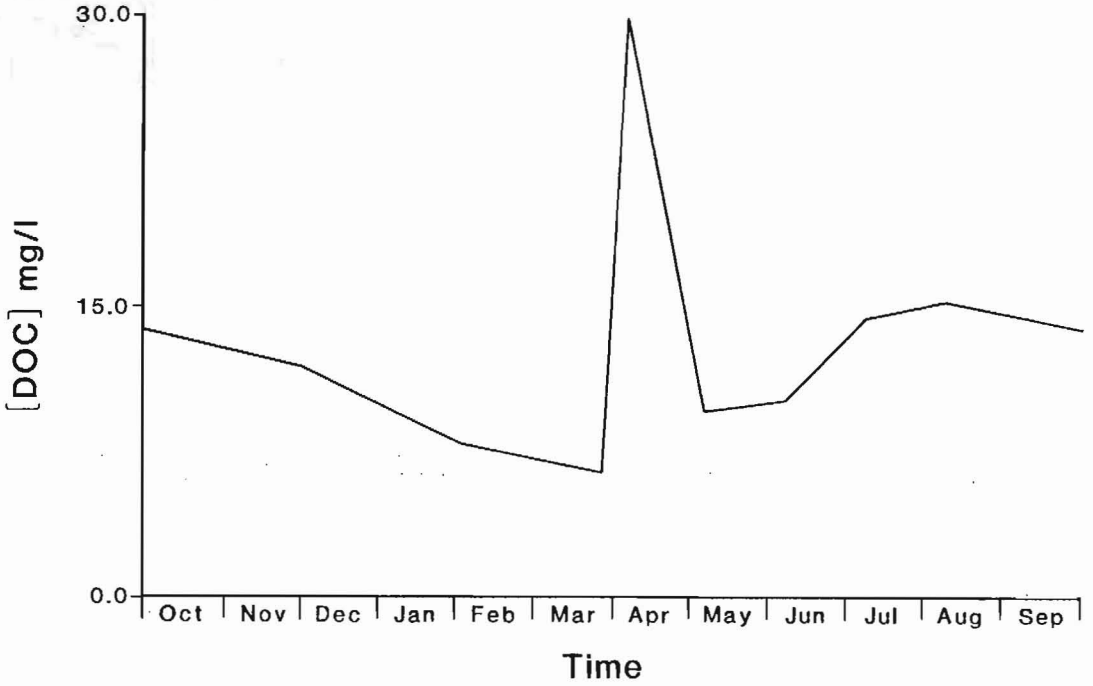


Figure 48. Simulated stream [DOC]--Filson Creek (1-year model run).

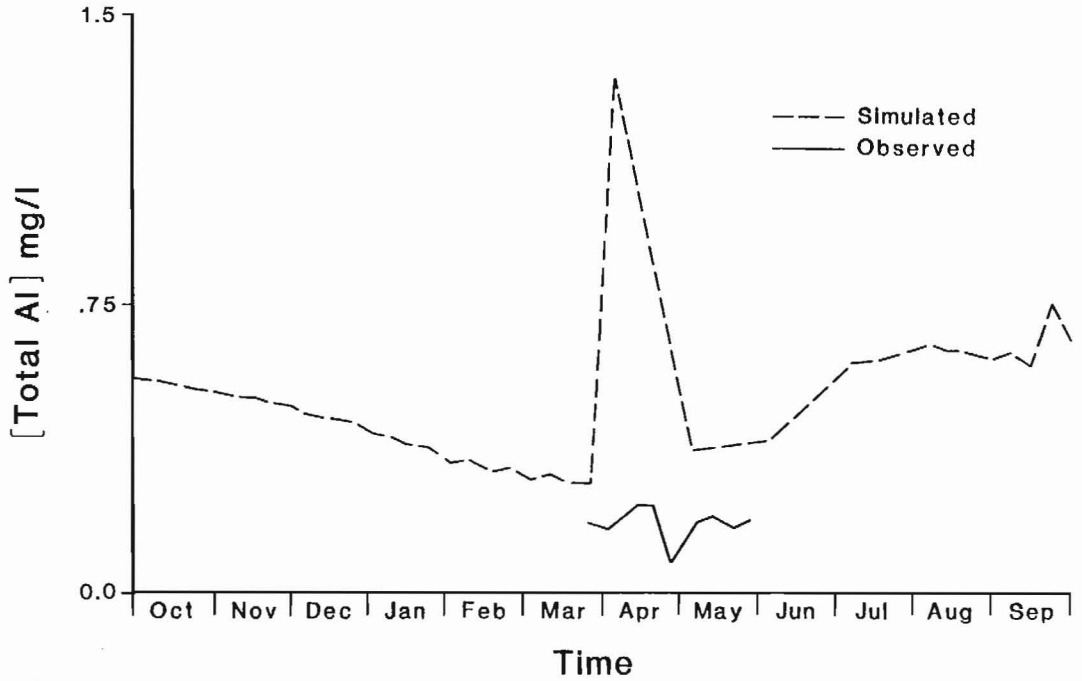


Figure 49. Simulated and observed [total Al]--Filson Creek (1-year model run).

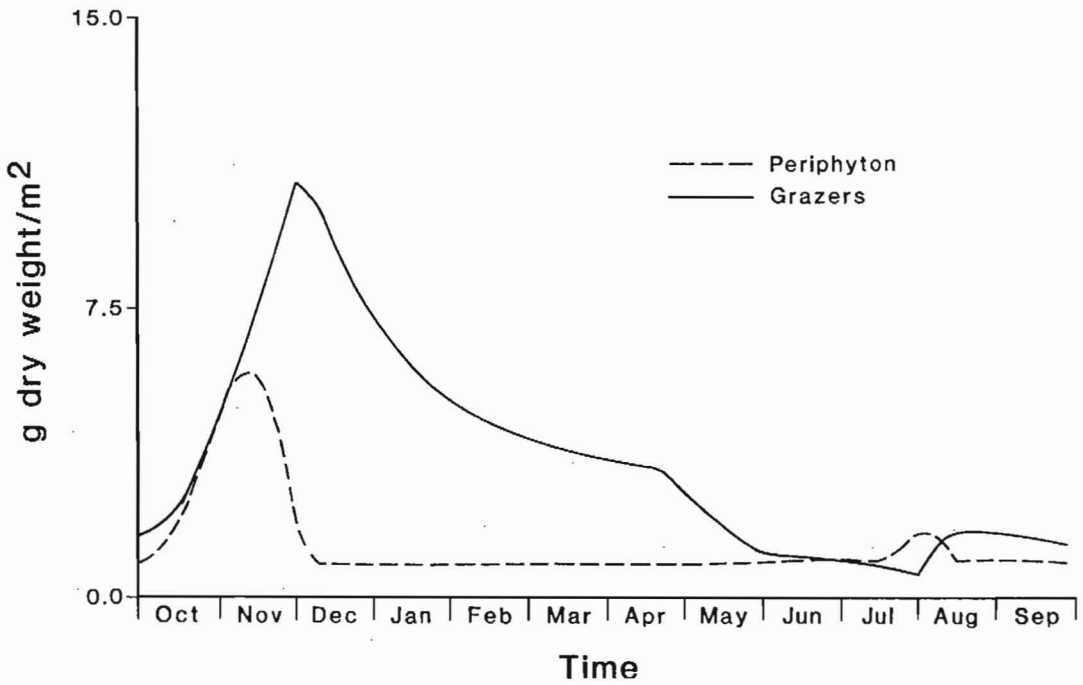


Figure 50. Simulated periphyton and grazers--Filson Creek (1-year model run).

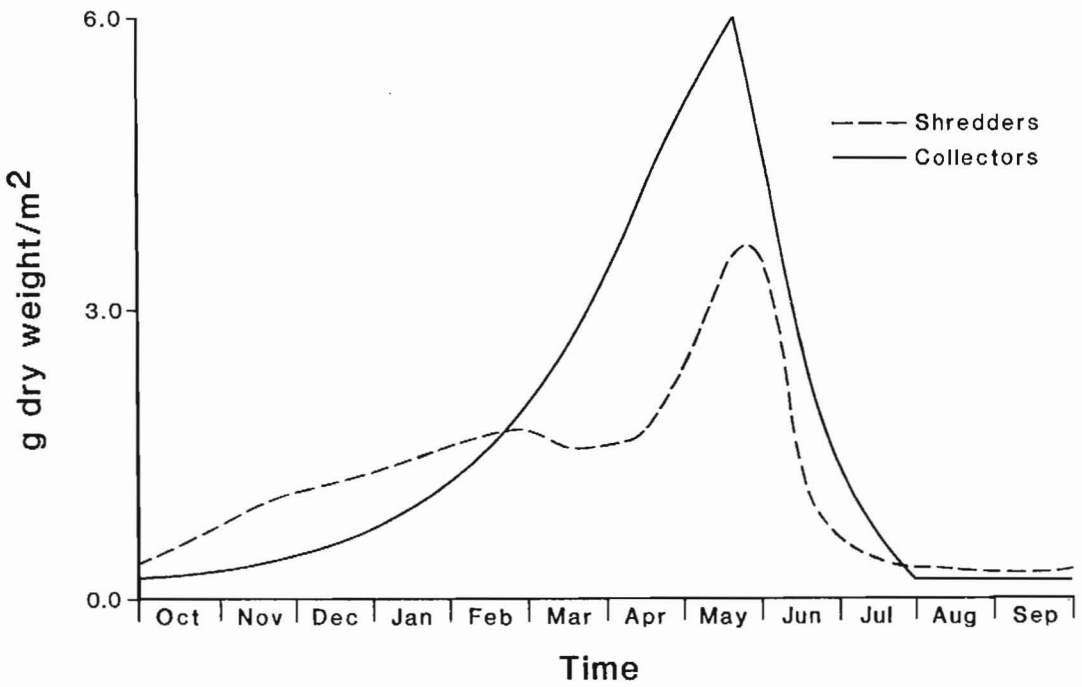


Figure 51. Simulated shredders and collectors--Filson Creek (1-year model run).

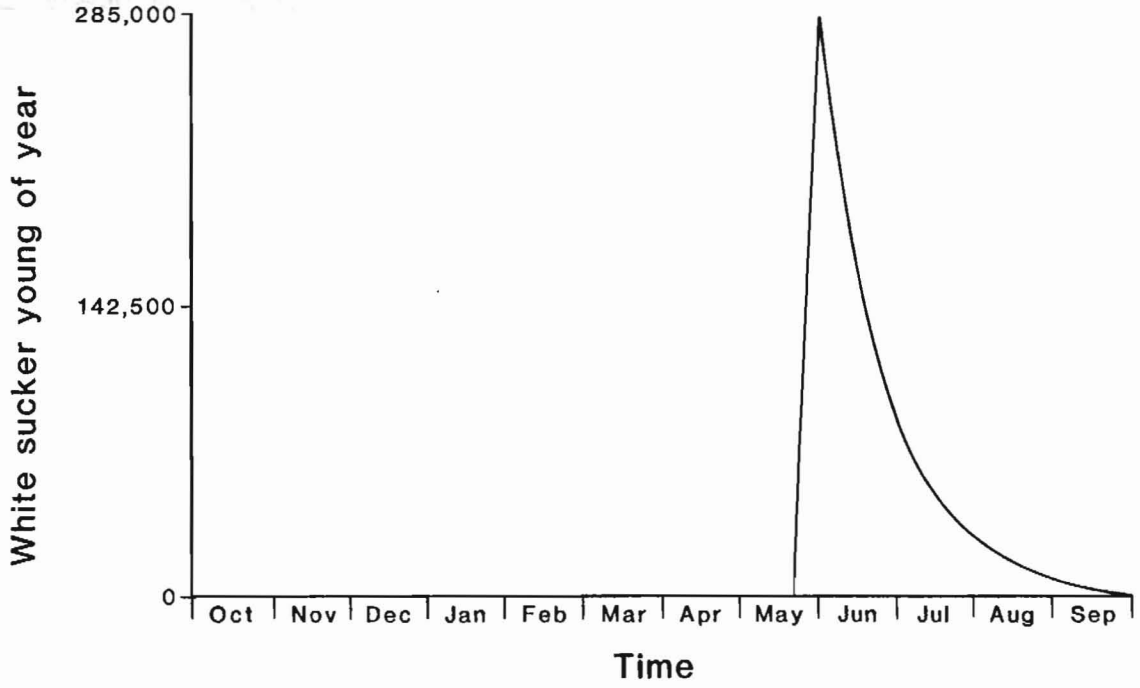


Figure 52. Simulated white sucker young of the year--Filson Creek (1-year model run).

10. MODEL LIMITATIONS AND RESEARCH NEEDS

Computer simulation models are abstractions of real world systems. The kinds of questions that are appropriate to address with a model depend on its degree of abstraction and level of refinement. The simulation model developed during this project was not intended to be a predictive management tool and, at its current level of refinement, use of the model for predictive purposes is inappropriate. Rather, the process of building and testing the model was used to provide a framework for addressing research needs and model refinements needed to adequately address the effects of acid precipitation on aquatic resources in different geographical areas. This process also helped identify interactions within the natural resource system for which the effects of acid precipitation are poorly understood. Attempts to parameterize and validate the model revealed limitations associated with model structure, as well as limitations in terms of available data bases.

The primary research need identified during the Acid Precipitation Workshop was for integrated watershed studies, spanning major abiotic and biotic components. Comprehensive studies providing all the data necessary for parameterizing and validating this or similar models have not been conducted. Several studies, however, provide relatively complete data bases (Likens et al. 1977; Scheider et al. 1979a, 1979b; Electric Power Research Institute 1981). In general, aquatic biota have not been considered in the selection of calibrated watersheds for ecosystem level studies. Some of the criteria and biotic information needs which should be assessed, along with physical features, when selecting sites for calibration include: (1) a fish community representative of species in the region; (2) the ability to control or measure human exploitation of the fishery; (3) the ability to control or measure emigration and immigration of the fish populations; and (4) the ability to monitor lower trophic levels on a seasonal basis. Integrated watershed data bases are essential to develop a better understanding of the effects of acid precipitation on aquatic resources and to refine and validate models enough to address management concerns with confidence.

Other research needs and model limitations identified during the Acid Precipitation Workshops concerned more specific aspects of model conceptualization and parameterization. These research needs are discussed with respect to the submodels developed during the workshops.

WATERSHED

The development of the Watershed Submodel raised a number of concerns about which factors are most important in determining the susceptibility of a lake to acidification. Watershed factors commonly identified in determining lake susceptibility include bedrock, watershed/lake surface ratio, lake elevation and regional terrain, and nature and thickness of soils. These criteria may be appropriate for some areas of North America, particularly the Adirondacks. However, somewhat different criteria may be required for Midwestern and, perhaps, Ontario watersheds.

Research designed to determine susceptibility factors should be expanded to address a larger geographical area and a broader spectrum of variables. Major watershed factors which should be addressed include the nature of acid deposition, watershed processing, and hydrologic regime.

Nature of Acid Deposition

The form of the acidic input was identified as one area which could be important in determining the amount of acid delivered to the receiving water. Determination of the relative amounts of SO_x and NO_x and the distribution of acid inputs between dry, gaseous, and wet forms were considered research areas that require further attention.

Watershed Processing

Geochemical processing. A variety of questions were raised during the workshops concerning important chemical reactions within the soil profile, including surficial geology. Important research needs in this area include

kinetics of soil reactions and the nature of soil leaching and exchange reactions, especially with respect to metals and cations. It is well documented that aluminum compounds contribute to fish deaths in Adirondack lakes. However, other metals, such as copper and zinc, may be leached in lethal concentrations in the quartzite sands in the northern lake States. The availability of various metals may be an important factor in acidification impacts. Another area considered important to address was the natural weathering rate and regeneration of cations.

Biological-organic processing. Terrestrial biological interactions between acidic inputs and lake acidification are poorly understood. Some of the identified research needs include the effects of acid on microbial activity, transformation of materials in the soil litter and organic layers, and the effect of organic material in bogs and wetlands in modifying watershed response to acidification. In particular, more information is needed regarding the complexing of organics with metal species. Research concerning the effects of vegetative cover in modifying atmospheric deposition should continue, but the relative importance of this mechanism in relation to changes within soil horizons appears to be relatively minor.

Concentration-discharge Relationships. Stream chemistry in this model is based on a set of regression equations which relate concentrations of water quality constituents to streamflow. These relationships are not usually available for watersheds and their development from available data is not necessarily straightforward. The regressions are only valid for the range of atmospheric loadings and watershed characteristics from which they were developed. The model does not mechanistically treat alteration of precipitation chemistry by the watershed, effects of changes in atmospheric loadings or watershed characteristics are, therefore, incorporated only indirectly as additions or subtractions to the regression results, based on assumptions concerning vegetative uptake and release. Although a mechanistic treatment of watershed chemistry would allow these changes to be addressed directly, the cost of parameterizing such a model would be very high and is probably impossible given current data bases.

Some water quality parameters exhibit a time-concentration response. This is particularly true for sulfate. Sulfate is a relatively conservative parameter that may be deposited in the watershed in gaseous and particulate form. If there is an extended dry period, a significant accumulation of sulfate may result. This accumulation will be leached from the watershed during a substantial rainfall. As a result, sulfate leaching is a function of the time period between rainfall events. This type of response is not directly incorporated into the model, although it is indirectly incorporated through the concentration-discharge relationships. Research is needed to better understand concentration-time relationships. This research needs to address threshold discharge values to produce sulfate leaching. In addition, the capacity of the soil and vegetation to retain sulfate needs further study.

Another limitation of the current model is the assumption that cation exchange capacity of the soil remains constant. In fact, the cation exchange capacity probably decreases through time during inputs of acid precipitation. This results in a loss of buffering capacity for the watershed and an increasing susceptibility to, and rate of, acidification.

Hydrologic Regime

The present simulation model is structured to represent a headwater stream/lake system typical of the Canadian Shield; for example, lakes in the Adirondacks and Ontario. These lakes are often situated in watersheds with considerable exposed bedrock, thin soils, and shallow glacial overburden. Many of these lakes are located directly over relatively impervious bedrock, and hydrologic regimes are primarily governed by surface runoff from the watersheds.

Glacial geology plays a much greater role in determining lake susceptibility in the Great Lake States of Minnesota, Wisconsin, and Michigan. Although portions of these States are situated over the Precambrian Shield, lakes are generally located over large amounts of glacial overburden, in some cases over 100 m in depth. Available data indicate that the thickness of glacial till (Electric Power Research Institute 1981) and relative contribution of ground water (Webster et al. 1981) determine lake susceptibility to acid

deposition for softwater lakes located within these glacial materials. Plotting calcite saturation index data (Kramer 1976) for lakes in northern Wisconsin (Webster et al. 1981) indicates that most of the susceptible lakes are seepage lakes (no surface inlets or outlets) (Fig. 53). Thirty-six percent of the 276 northern Wisconsin lakes sampled were susceptible to acid deposition (Fig. 54). Based on this criterion, approximately 2,600 northern Wisconsin lakes are susceptible to acidification. A similar number of lakes in northern Minnesota and upper Michigan are expected to be susceptible, assuming there are no substantial differences in the nature of the glacial overburden between States.

Ground water is commonly determined as the residual in the hydrologic budget. This does not appear to be a satisfactory approach for detailed analyses of lake acidification. The interchange of ground water with surface water can be estimated using the LaPlace equation when the stratigraphy and potentiometric surface of the surficial aquifer are known. The effect of nonsteady conditions in modifying the annual average ground water influence on the lake alkalinity budget can be addressed using a more complex time-variable model, provided adequate field data are available for calibration. Including ground water as a measured component in the hydrologic budget also makes it possible to estimate ground water residence times (an important factor when addressing natural weathering), regeneration of cations, and kinetics of other important chemical reactions in the watershed.

WATER CHEMISTRY

The Water Chemistry Submodel was not designed to address complex solution chemistry in a rigorous way. However, the present computational approach should be sufficient for simulating a wide range of water quality conditions as a basis for assessing biological responses. A number of important research needs were identified during development of the current computational approach and associated discussions of more detailed solution chemistry.

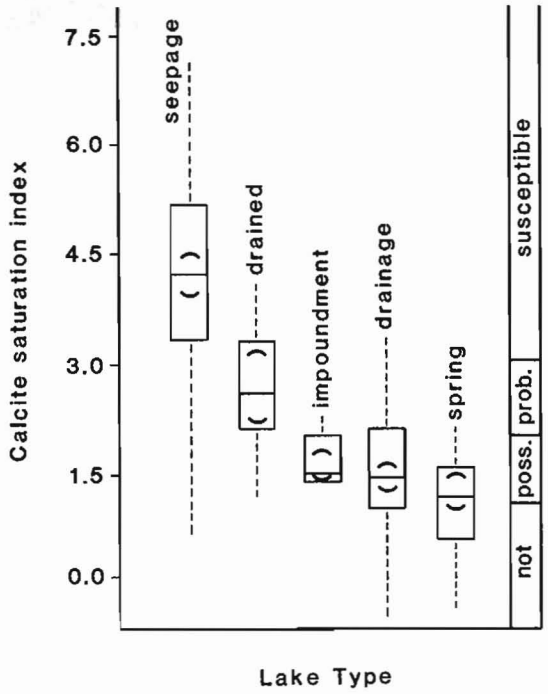


Figure 53. Boxplots of calcite saturation index according to lake type for 276 northern Wisconsin lakes (from Webster et al. 1981).

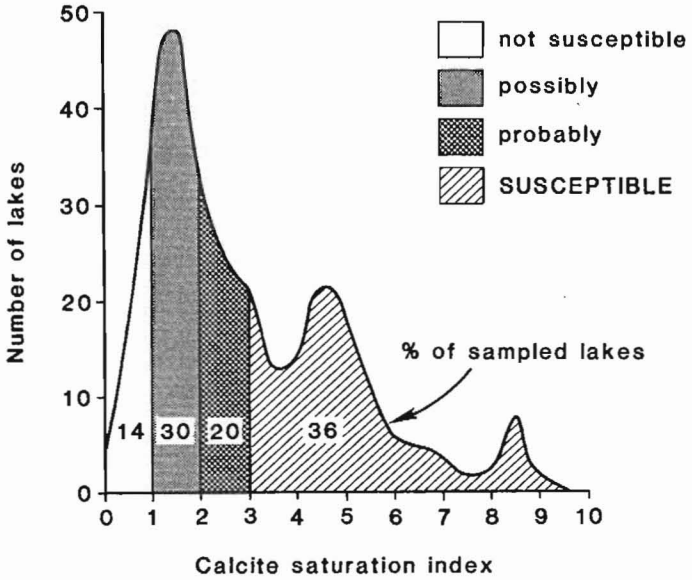


Figure 54. Distribution of calcite saturation index values for 276 northern Wisconsin lakes (from Webster et al. 1981).

Aluminum Chemistry

Aluminum hydrolysis. The Water Chemistry Submodel assumes equilibrium with respect to aluminum. This may be realistic over a long time range but not during conditions of rapid pH changes. Information is needed concerning the kinetics of aluminum and the fate of hydrolyzed aluminum in hydrolysis. This is particularly important because fish are susceptible to supersaturated levels of aluminum.

Ligand-hydrous aluminum oxide associations. Hydrous aluminum oxides are particularly good adsorbents at low pH levels. They may strongly influence the chemistry of aqueous anions, such as organic acid (DOC), orthophosphate, sulfate, and fluoride. Organic acid and orthophosphate levels are particularly significant with respect to algae dynamics. Water color associated with organic acids decreases as organic acids are adsorbed on hydrous aluminum oxides. The concomitant increase in light penetration can increase primary production in the lake. Phosphorus-hydrous aluminum oxide associations, on the other hand, generally result in decreased phosphorus levels, thereby decreasing algae growth and the associated generation of base equivalents.

Ligand-aqueous aluminum associations. Ligands, such as fluoride and organic acids, may significantly influence dilute system chemistry, in part through aluminum complexation reactions. Fluoride and organic acids form very strong complexes with aqueous aluminum and, therefore, may significantly mobilize this element. The relative role of hydrogen ions, fluoride, and organic acids in the regulation of aqueous aluminum needs to be studied.

Speciation and Ligand Associations of Trace Minerals

Metals, such as aluminum, zinc, manganese, and copper, are potentially toxic to organisms in dilute water systems. Speciation of these metals generally influences their toxicity to organisms. A better understanding of metal forms is needed in order to evaluate toxicity potential.

Role of Organic Acids

In addition to chelation reactions discussed previously, organic acids may serve as proton donors in water chemistry. Organic acids could, therefore, potentially contribute to the acidity of the aquatic environment. More information is needed on the role of organic acids in lake acidification.

Sediment Influence

Chemical reactions within the model are assumed to take place in the water phase. This necessary assumption ignores the potentially important, but poorly understood, contribution of sediments in modifying nutrient cycling, toxicity of metal forms, and buffering capacity in dilute water systems. Mechanisms through which sediments can influence water chemistry include sediment exchange reactions, sulfate reduction reactions, and turbulent diffusion of chemical constituents up into the water column.

Sediments serve as important exchange sites for metals that occur in elevated concentrations in acidified systems. The composition of sediments, particularly the relative amount of clay and sand, may radically affect the ability of individual systems to mobilize toxic metals into the water column. The amount of clay, sand, and organic matter also affects the buffering capacity of sediment. Failure to account for this buffering can result in an underestimation of total buffering capacity of the lake system, resulting in an overestimation of the rate of lake-stream acidification.

Lake Stratification

The Water Chemistry Submodel assumes complete mixing in the lake; therefore, potentially important effects of stratification (temperature and water quality) on aquatic biota are not included. These effects are discussed under Plankton-Benthos and Fish Submodel limitations and research needs.

Management Strategies

Chemical additions (base or nutrient) should be investigated as management strategies. Liming or phosphorus additions are not generally done in a cost-effective manner at this time. A rational procedure for computing chemical dosages should be developed. Calculations should consider aluminum-phosphorus interactions, as well as nonhydrogen ion-inorganic carbon sources of aqueous acidity, such as aluminum and organic acids.

PLANKTON-BENTHOS

Classical treatments of food chain kinetics have been primarily concerned with energetics and nutrient limitation. An acid precipitation model must also evaluate the impact of increased toxicity and the influence of pH changes. This relatively new approach in biological analysis highlights serious gaps of knowledge which limit the development of predictive models suitable for management application. Some knowledge deficiencies are common to all trophic levels. Acidity influences species diversity and community composition. These shifts can result in changes in the palatability of food sources to various predators. The model, however, assumes that this does not happen. The effects of acidity on the process rates (e.g., respiration, grazing, and photosynthesis) of aggregated functional groups is critical to the behavior of the Plankton-Benthos Submodel; these aspects are poorly represented in the model and poorly understood. These areas are important research needs which must be met in order to address the effects of acid precipitation with a feasible mechanistic approach. In addition, possible compensatory responses of biological communities impacted by acidification and concurrent mobilization of metals are not yet experimentally defined.

Lacustrine

Several simplifications and assumptions were made during the formulation of the Plankton-Benthos Submodel. In order to make this submodel applicable to a variety of lakes, the lake may need to be described in terms of vertical

segments. This requires knowledge of the pattern of thermal stratification and hydrodynamics of the water column. Processes that are potentially critical, but remain undocumented, were necessarily omitted. Experimental approaches which characterize the following functional elements are especially needed.

Phosphorus. Quantifying the pH-dependence of phosphorus release from lake sediments, as well as coprecipitation phenomena and adsorption with regard to phosphorus-aluminum interactions, are of paramount importance. Specific rate coefficients for decomposition processes and nitrate and phosphorus recycling are needed relative to temperature and pH at each recycling step. Ratios of unavailable:available phosphorus partitioned during recycling need to be defined with reference to both temperature and pH, according to suspected compensatory responses. Clearer definition of phosphorus uptake by phytoplankton versus scavenging of phosphorus by pH-dependent chemical kinetics requires detailed examination. Terms denoting the contributions to each phosphorus pool via fish, zooplankton, and benthos excretion should be parameterized.

Phytoplankton. Very little is known about the influence of pH on basic physiological processes in phytoplankton. Interactive influences of temperature and pH need clarification relative to species-specific growth rates and their influence on phytoplankton community composition (species abundance). Direct influence of acid on photosynthetic capacity and phytoplankton respiration is likely. Species-specific reductions in phytoplankton biomass due to differential grazing by small and large zooplankton are incompletely understood. The trophic dynamics modeled here must be redefined if phytoplankton community composition shifts so that algae biomass is composed of species unavailable or unpalatable to zooplankton. A precise formulation is needed for changes in the attenuation of light due to lake color, a common phenomenon in many susceptible lakes, and its subsequent influence on primary production which supports the food chain. Analytical interferences due to dissolved organic compounds common in colored waters require special attention, especially when determining chlorophyll-a concentration.

Zooplankton and benthos. The functional responses of zooplankton and benthos to acidity need precise definition. Threshold levels of response and their functional form must be determined to accurately model impacts. Information on size-frequency distributions within zooplankton and benthos communities needs to be cataloged, along with documentation of shifts in distribution under acid stress and associated changes in water chemistry. Size-specific predation rates by fish under increasingly acidic circumstances need further clarification. The influence of acid and temperature, and their interactions, on the feeding and energetics of all size classes of common species within each community must be investigated in order to characterize species-specific acid impacts on reproductive output and community production. The identification of the relative physiological sensitivity of various species may lead to the identification of indicator species that can be used in determining the level of ecological impact.

The benthos element of the lacustrine Plankton-Benthos Submodel is dealt with by dividing the benthos into two size categories, both of which are subject to predation by fish. This simplification may be realistic for addressing the effects of acidification on fish, but obviously ignores the complexity of benthic communities. The lake benthic community is represented in the model as a single trophic component. In reality, several functional groups are present, including decomposers, detritivores-scavengers, filter feeders, predators, and primary producers. Differential effects of acidification on important organisms within the functional benthic groups can change the mechanism by which aquatic biota are impacted. For example, species replacement, such as that observed with *Sphagnum* dominance in some acidified lakes, may cause major alterations in nutrient recycling.

Lotic

The lotic Plankton-Benthos Submodel requires many parameters for which available information is limited. This restricts the applicability of the model. Many of the more general research questions identified in the previous lacustrine section are also relevant to lotic systems. In particular, it is necessary to know effects of the altered chemical components on the food chain

groups and their processing rates. Moreover, the relationship between water chemistry and the decomposition and conditioning rates of allochthonous inputs must be understood, because the detrital food chain is usually the principal source of energy to the stream biota.

FISH

The Fish Submodel incorporates as much realism as possible. Although a more sophisticated conceptual design might be desirable, a lack of the necessary data prevents this approach. However, construction of the submodel helped to identify data requirements and research needs for future modeling efforts.

Potential Compensatory Responses to Acidification

Impacts of acidification on aquatic organisms are assumed, for modeling purposes, to result from toxicity caused by ambient hydrogen ion-aluminum concentrations or changes in total abundance of food at a lower trophic level. However, some organisms are known to adapt and survive in highly acidic lakes and streams.

Population responses, including shifts in age at maturation, changes in fecundity, density-dependent mortality rates, and the occurrence and relation of intermittent iteroparity to stress need to be investigated. Genetic relationships requiring additional information include selection for increased physiological tolerance to acid-aluminum stress and selection for fish stocks with life history patterns compatible with acidification patterns (e.g., late versus early spawners).

Other responses of fish acidification include adaptations in temporal or spatial factors. For example, fish species which spawn after spring runoff avoid high concentrations of acid snowmelt. Such variations and adaptations in the time of spawning are not incorporated in the Fish Submodel. The extent

to which such adaptations occur in acidifying stream-lake systems needs to be evaluated. In lakes with multiple inlets, certain species of fish may avoid spawning in the more acidic inlets, ensuring reproductive success despite the input of highly acidic runoff to the lake. The present model assumes only a single inlet and may, therefore, overestimate impacts on reproductive success. The present model also does not allow for movement of fish into or out of the lake through the outlet stream. This omission may not be a serious deficiency when assessing the net impact of acidification on the resource, but could cause errors in determining rates and mechanisms of reductions in fish populations.

The model also assumes instantaneous complete mixing within the lake; therefore, additional differential spatial impacts are not addressed. For example, snowmelt runoff is generally less dense than lake water and, consequently, highly acidic runoff may stratify on the lake surface. This likely results in greater damage to organisms in the littoral zone. In the profundal zone of acidified lakes, Chironomidae often become dominant. This may reflect the organisms' close association with sediments which probably act as a buffer. Much of the biological community in streams is either associated on, or within, the streambed. This connection between the stream community and the substrate may result in very different responses of biological communities in streams from those in lakes.

Bioenergetics

Research and model refinements needed in the area of bioenergetics include the effects of acidification, temperature, and starvation stress on the partitioning of energy for growth, reproduction, and metabolism and secondary consequences for food chain energy transfers. More information is needed on interactions among fish species, in terms of competition for food resources, predation, and social behavior in habitat interactions. Field studies to determine physiological indicators of acidification-induced stress are needed.

Mortality Functions

The application of fish mortality functions from Baker's (1981) thesis needs to be qualified. These data, although clearly the best and most comprehensive available at this time, remain subject to application problems. Baker relates mortality of various life stages of white sucker and brook trout to manipulated values of pH and aluminum. Regression models were derived under experimental conditions where temperature, calcium, and duration of exposure were fixed. The effects of varying calcium levels and temperature on model response need to be evaluated. The effect of long term exposures of these fish species to these factors must be known to determine limits for adaptive response. Also, speciation of aluminum under experimental conditions differs significantly from field situations. For example, potentially toxic inorganic fractions in the field include F- complexes which are of lower toxicity and have not been considered in experiments. The rate of change in pH and Al also alters dose-response functions but is not accounted for in the regressions. In addition, the regressions may not be applicable to fish species other than white sucker and brook trout and do not account for biological variation within each species. As an example of possible biological variation, comparison of molluscs in New York and Wisconsin indicated that the minimum tolerable pH value for the same species can vary by as much as one pH unit. Finally, these mortality functions were developed for pH-aluminum toxicity, while metals, such as copper and zinc, may be of greater importance in other geographical areas.

Chronic Effects

The chronic effects of acidification, which are not well documented, include the inhibition of gametogenesis, repeated recruitment failure and its impact on population age structure and biomass, and physiological alterations or chemical changes in signal substances in terms of olfactory responses in homing species.

Management Strategies

The model should incorporate several management considerations, such as: stocking of resistant species; introductions of non-native species (e.g., yellow perch); provision of alternative spawning sites through activities such as reclamation of spawning habitat and nursery areas destroyed or impaired by logging, natural catastrophies, or beaver activity; lake reclamation (e.g., rotenone application) to eradicate unwanted species and subsequent introduction of desirable species; and regulations, such as size and creel limits or changes in land use or access.

SUMMARY

The research needs related to acid precipitation discussed in this chapter do not represent an exhaustive list of potentially useful research. They do represent the best judgement of the workshop participants about the most important needs for a better understanding of the acidification process and its effects on aquatic resources. Results from this research will help improve strategies for addressing problems related to acid precipitation and will be useful in future modeling efforts.

Current computer simulation models of the acidification process and its effects probably do not have sufficient predictive power to be used directly in evaluating management strategies. However, models, such as the one developed during this project, do provide a framework for integrating existing knowledge and a holistic perspective of changes in watershed ecosystems that are the result of acid precipitation. The increased understanding which comes from this holistic perspective can be used to develop strategies for addressing acid precipitation problems. For example, FWS biologists are becoming increasingly involved in assessing potential impacts of acid precipitation on fishery resources. However, the model demonstrates that fisheries resources are a subset of interconnected biotic and abiotic components and processes which make up a watershed ecosystem. Answering questions about the effects of acid

precipitation on fish resources consequently requires an interdisciplinary approach. Therefore, particular care should be taken to develop a fish and wildlife research strategy that recognizes and addresses these interdisciplinary links.

As our knowledge of the acidification process and biological responses increases, models can be built that more accurately represent the important processes and interactions. These models will be more useful, in a predictive sense, for tracing the effects of acid precipitation through a watershed ecosystem and for addressing potential management strategies. Models, however, will remain incomplete representations of real world systems and, as such, should be only one of the tools used to make management decisions.

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APPENDIX
AEA Acid Precipitation Workshop Participants

Anders Andren
Department of Water Chemistry
University of Wisconsin
Madison, Wisconsin 53706

Larry Barnthouse
Oak Ridge National Laboratory
Environmental Sciences Division
P.O. Box X
Oak Ridge, Tennessee 37830

Jay Bassin
Office of Biological Services
U.S. Fish and Wildlife Service
Washington, D.C. 20240

James Bennett
National Power Plant Team
U.S. Fish and Wildlife Service
2929 Plymouth Road, Room 206
Ann Arbor, Michigan 48105

Kenneth Biesinger
Environmental Research Lab.-Duluth
6201 Congdon Blvd.
Duluth, Minnesota 55804

Wes Bradford
USGS
National Center, MS-412
Reston, Virginia 22092

Dave Brakke
Huxley College
Western Washington University
Bellingham, Washington 98225

Thomas Burton
Michigan State University
Institute of Water Research
East Lansing, Michigan 48823

Patricia Carstensen
National Power Plant Team
U.S. Fish and Wildlfe Service
2929 Plymouth Road, Room 206
Ann Arbor, Michigan 48105

Lee Conway
Brookhaven National Laboratory
Department of Energy and Environment
Building 318
Upton, New York 11973

Ellis Cowling
School of Forest Resources
North Carolina State University
Raleigh, North Carolina 27650

Peter Daye
Daye Atlantic Salmon Corporation
P.O. Box 1081
Armdale, Nova Scotia
Canada B3L 4L5

Charles Driscoll
Civil Engineering Department
Syracuse University
150 Hinds Hall
Syracuse, New York 13210

Joe Eilers
Wisconsin Department National Resources
232 Scheik Plaza
Box 818
Rhinelander, Wisconsin 54501

Ron Eisler
Office of Biological Services
U.S. Fish and Wildlife Service
Department of Interior
Washington, D.C. 20240

Robert E. Foley
New York Dept. of Environ. Conservation
Hale Creek Field Station
7235 Steele Avenue Ext.
Gloversville, New York 12078

Robert Friedman
Office of Tech. Assessment
U.S. Congress
Washington, D.C. 20510

Eugene Fritz
National Power Plant Team
U.S. Fish and Wildlife Service
2929 Plymouth Road, Room 206
Ann Arbor, Michigan 48105

Terry Haines
CNFRL-Field Research Unit
U.S. Fish and Wildlife Service
University of Maine
Orono, Maine 04473

Jack Hargis
University of Minnesota
Department of Biology
Duluth, Minnesota 55812

Dale Hoffman
U.S. Fish and Wildlife Service
Division of Environment
P.O. Box 25486, DFC
Denver, Colorado 80225

A. J. Johannes
Dept. Chemical and Environmental
Engineering
Rensselaer Polytechnic Institute
Troy, New York 12181

Richard Johnson
U.S. Fish and Wildlife Service
2625 Redwing Road
Fort Collins, Colorado 80526

Arnold Julin
U.S. Fish and Wildlife Service
One Gateway Center, Suite 700 (AEV)
Newton Corner, Massachusetts 02158

William Kovalak
H-124 WSC-Detroit Edison
2000 Second Avenue
Detroit, Michigan 48226

Dave Lenhart
U.S. Fish and Wildlife Service
Lloyd Building, Suite 1692
500 NE Multnomah Street
Portland, Oregon 97232

Rick Linthurst
North Carolina State University
Department of Botany
P.O. Box 5186
Raleigh, North Carolina 27650

Orie Loucks
Science Director, The Institute
of Ecology
4600 Sunset Blvd.
Indianapolis, Indiana 46208

C. David McIntire
2025 NW Elder Stree
Corvallis, Oregon 97330

Richard Miller
Professor of Zoology
Butler University
4600 Sunset Blvd.
Indianapolis, Indiana 46208

Rufus Morrison
Office of Research Development
EPA
401 "M" Street, SW
Washington, D.C. 20460

Gordon Omen
University of Minnesota-Duluth
Department of Physics
Duluth, Minnesota 55812

Charles Powers
Environmental Protection Agency
CERL-200, SW 35th Street
Corvallis, Oregon 97330

Paul Rago
Great Lakes Fisheries Lab.
1451 Green Road
Ann Arbor, Michigan 48105

Paul Rodgers
DePaul-LLRS
9311 Groh Road
Grosse Ile, Michigan 48138

Tom Roush
Environmental Research Lab.-Duluth
6201 Congdon Blvd.
Duluth, Minnesota 55804

Wolfgang Scheider
Ontario Environment
P.O. Box 213
125 Resources Road
Rexdale, Ontario Canada M9W 5L1

Jerry Schnoor
Environmental Engineer
University of Iowa
Iowa City, Iowa 52240

Carl Schofield
Cornell University
Department of Natural Resources
Fernow Hall
Ithaca, New York 14853

Kent Schreiber
U.S. Fish and Wildlife Service
EELUT, NPDG
Route 5, Box 44
Kearneysville, West Virginia 25430

Stan Smith
U.S. Fish and Wildlife Service
538 Federal Bldg. and U.S. Court House
316 North Robert Street
St. Paul, Minnesota 55101

Jim Weiner
Leader, Field Research Station-LaCrosse
P.O. Box 936, 2630 Fanta Reed Road
LaCrosse, Wisconsin 54601

Monta Zengerle
EPRI
3412 Hillview Ave., P.O. Box 10412
Palo Alto, California 94303

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