Proceedings International Symposium on the Design of Water Quality Information Systems

DESIGN OF WATER QUALITY INFORMATION SYSTEMS

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PREFACE

Understanding the behavior of environmental variables is a prerequisite to society's efforts to manage the environment in an effective and efficient manner. Since the 1700s, when many of our current scientific approaches to studying environmental variables were first formulated, the goal has been to recognize patterns in behavior that help society understand and manage these processes. Durant, in his history of civilization, notes that during the 1700s "science strove to detect regularities in the vagaries of weather. The first requisite was reliable records." Today we continue to try to understand our environment and we continue to need reliable records as well as data analysis methods that convert the data to information that advances our understanding.

This effort to gain more understanding of our environment and its behavior received a major boast during the 1960s and 1970s as society's impacts resulted in several major environmental "catastrophes" that received wide publicity. With each "catastrophe," there appeared a new law to address that specific problem in our society, especially in the U.S. where a rather legal approach to environmental management was utilized. As the number of laws, agencies, personnel, treatment plants, and environmental impact statements increased, the environmental problems did not seem to go away, even though there have been some notable successes (e.g. Lake Erie and the Potomac River). In recent years, it seems that science has identified new environmental problems faster than society can solve the old ones.

Simply passing laws and spending large sums of money to clean up old problems will not permit society to protect the environment. Effective management requires a fundamental understanding of what the quality of the environment is and why it is that way.

This recognition is causing many elements of society to now reexamine what was previously viewed as an adequate understanding of the behavior of environmental variables. This is especially true in water quality management!

As the public, its elected representatives, and environmental managers seek to know what the quality of water is and why it is that way, the need for better information on the behavior of water quality variables in the environment is recognized. The means by which this information is obtained is not readily clear, as the environment is a mixture of complex processes that determine the quality of water. Many traditional means of "water quality monitoring" grew out of the need to simply "monitor" compliance with legal standards without really trying to quantify an understanding of the what and why of water quality.

As professionals in water quality monitoring attempt to shift their monitoring efforts from a compliance only format to one of obtaining a better understanding of the behavior of water quality variables in the environment, they offer no established body of literature which can be used to direct the redesign or reformulation of their approaches to monitoring.

Colorado State University, following its long history in developing measurement procedures and data analysis methods in the field of water resources, has had research and teaching efforts underway in water quality monitoring for the past 20 years. In 1979 a short course on the design of water quality monitoring networks grew out of these research and teaching efforts. By the mid 1980s it became clear to many at Colorado State that it was now time to begin pulling a body of knowledge together that could be readily accessed by water quality monitoring

professionals to assist them as they refocused their monitoring efforts from simple-data collection to meeting specific information needs on water quality variable behavior. U.S. Environmental Protection Agency personnel were very supportive of efforts by Colorado State faculty in attempting to bring together monitoring design information.

On 7-9 June 1989 an International Symposium devoted solely to the design of water quality "information" systems was held in Fort Collins, Colorado. The Symposium was sponsored by Colorado State University and the U.S. Environmental Protection Agency. By using the word "information" in the title of the Symposium, the organizers hoped to focus water quality monitoring away from data as an endpoint and indicate a larger purpose focused on water quality information. Thus, the Symposium was designed to bring together environmental scientists, engineers, managers, and statisticians concerned with utilizing monitoring to develop a better understanding of the behavior of water quality variables in the environment. While water quality monitoring involves a number of "steps"-- sampling, laboratory analysis, data handling, data analysis, reporting, and, ultimately, utilization of the information, the Symposium emphasized the "information" end of the system (the last three steps).

The Symposium focused on determining how water quality monitoring efforts could answer the questions: "What is the quality of the water?" and "Why is the quality of the water what it is?" The goal was to determine how monitoring can provide information that could be used to answer specific management questions.

The attendees, being focused on the rather narrow topic of water quality information systems, created a dynamic and stimulating discussion of the subject. Hopefully, these proceedings capture the essence of the presentations made 7-9 June 1989.

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Opening Session

WELCOME

Neil S. Grigg, Director
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We are pleased to have you at Colorado State University to attend the conference on Water Quality Information Systems. CSU is a leader in the international water resources field, and the convergence of the two subjects of water quality and information systems is critical for the future of water resources management.

From my own background on water quality management, I have considered what some of the important problems related to monitoring are. It's not a complete list, but here are some problems that impress me with their importance and difficulty:

(1) How do we measure micro-contaminants to show the full effect on ecosystems of different kinds of human activities? The microcontaminants are difficult to measure as the size and diversity change, and even if we can measure them, we don't always know the health or the ecosystem effects. We need more emphasis on biomonitoring.

(2) Is the job of environmental monitoring becoming too expensive? We need new approaches to integrate information and to optimize the use of networks, such as in estuary water quality monitoring.

(3) How do we reconcile the different economic abilities to provide environmental monitoring? Consider the difference between the U.S. and Africa, where the economic ability to provide sophisticated scientific input or instrumentation is vastly different.

(4) Even after the information is collected, how do we manage it? Processing environmental information to lead to manage-

ment decisions is the bottom line, an we can reliably and consistently mai data and analyze it to produce information, is it really worthwhile?

(5) Whose responsibility is it to n In the case of estuaries, EPA, NOAA state government and even citizen n are responsible for data collection.] we coordinate this large and massive

What is the purpose of monitoring. I believe there is a three-part purpos The information system is only valu part of a water quality management The management system must begin understanding of what is going on system. This is the first purpc monitoring: to increase our underst The second purpose of monitoring is t us to process information leading to de This is the decision-support system as monitoring, and in this modeling can useful. Finally, the purpose of monitc seen in actions that are taken to cl water. Monitoring can be used to rationale for the actions as well as to up to see the results of the actions.

With such an important topic, we h Colorado State to participate in resear education into the future. Colorado Sta a long history of involvement in resources management. We started i 19th century with emphasis on irri engineering, which has been made fam development such as the Parshall Flum other contributions by scientists su Robert Glover, who developed u approaches to ground and surface management. In more recent years, we

been known for our contributions in hydraulic engineering and the hydrologic sciences as well as our work overseas, such as international irrigation projects in Asia. Now, some of the water quality work that we are doing, such as the research on design of water quality monitoring systems, offers promise to lead us into the future.

Colorado State has an interdisciplinary approach to water resources education. The Departments of Agricultural and Chemical Engineering, Civil Engineering and Atmospheric Science represent the College of Engineering's approach to water; but we also have a strong natural resources component which includes the Departments of Fishery and Wildlife Biology, Earth Resources and Recreation Resources in the College of Forestry and Natural Resources. In Agriculture, we have Agricultural and Resource Economics and Agronomy, which are strong inputs to our total water resources program. The Colorado Institute for Irrigation Management and the Colorado Water Resources Research Institute, which I represent, are also important organizational vehicles.

Again, welcome, and if we can do anything for you here at Colorado State University while you are here for this conference or later, please let us know.

OPENING REMARKS

Robert C. Ward
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An "Information" Symposium in water quality!?! What does this mean? What is the Symposium going to cover?

I heard comments like this many times during the planning and execution of this Symposium. What is the background is such a Symposium?

I thought I would use my introductory remarks to provide a little background on the Symposium, and more broadly, on the general subject of information in water quality management.

Anyone who has designed and operated a water quality monitoring system knows that collection of data is the easiest part of obtaining information about water quality variables in the environment. Most monitoring systems operate relatively smoothly the first few years of their life as there is little analysis that can be done and the enthusiasm for the effort is high among those paying for the monitoring (or information gathering effort). After several years (maybe shorter), budgets get tight and the tough questions begin to be asked.

What are we getting for the money we spend on monitoring?

What happens if we reduce the monitoring budget by 20%?

Why do we monitor water quality?

And then the most threatening question of all is:

What is the quality of the water?

To me these types of questions, and our inability to quantitatively answer them, is the reason for this Symposium. There should b a well defined information product produce from every water quality monitoring effor Thus, we want to design not just monitoring program, but rather a wate quality informa- tion system that has a wel defined informa- tion product that permits th operation of an efficient and effective wate quality manage- ment program. If such wate quality informa-tion products were associatec with every water quality monitoring effort, th type of questions noted above would be askec much less fre- quently; and when they wer asked we would have ready, quantitativc answers for them.

What do I mean by water qualit "information product?" I'm not sure I car answer that question! What information about the behavior of water quality in the environment, do we need to manage water quality efficiently and effectively? Naisbitt, in his 1982 book entitled Megatrends, describes how our society is evolving into an information society and points out that "uncontrolled and unorganized information is no longer a resource in an information society. Instead it becomes the enemy of the information worked ... Information technology brings order ... and therefore gives value to data that would otherwise be useless." Jim Loftis, Graham McBride and I, in a 1986 paper entitled "The data-rich but information-poor syndrome in water quality monitoring" bring Naisbitt's observations to bare on the water quality information problems.

Why does water quality management today collect lots of data without a clearly defined use for the resulting information? I believe we have general uses for the data and resulting information in mind when we set up monitoring programs. ("In mind" is not

quantitatively design the means by which we will convert the data into the information we want. Also we rarely document, in writing, the monitoring system design.

If we were to try to document a quantitative design, I'm afraid that we would have very little guidance from the literature. Water quality management simply has not evolved to the point where the decisions that have to be made can always be defined in a quantitative manner. In addition, our understanding of the processes that we are trying the control in the environment is still evolving rapidly. As we gain a better understanding, we realize that the monitoring system we designed five years ago is already out of date and the data less useful than we had originally envisioned.

The program for this Symposium tends to focus on how to get data and analyze the data to obtain statistical results. Is this information? It is if its use within management is defined. I'm afraid that too often we produce statistical results (which is a lot better than producing data alone), but we still have a long way to go in developing a clear picture of what information we are to be producing for water quality management decision making.

How has this Symposium been developed and organized? Water quality monitoring can be viewed as a system through which the flow of water quality information is developed. One interpretation that I have used in the past is:

> Sample collection
> Laboratory analysis
> Data handling
> Data analysis
> Reporting
> Information utilization

The first three components have received relatively consistent attention for a number of years, and our success in their operation creates the large "data-rich" situation. The last three components, however, have not received much attention until recently, and our lack of attention here results in the "information-poor" situation. I have been par-

ticularly impressed by the advancements made in the area of data analysis over the past five to ten years. You will see and hear about many of the advancements during the Symposium.

We are working on the concepts of reporting within a water quality management program; however, I'm not sure how far we will get until we attack the last component-- information utilization. How do we make water quality management decisions, what are those decisions, and how does information on the behavior of water quality variables influence those decisions? As we go through the next few days, I hope we can address some of these issues in our individual conversations and, perhaps, begin to develop future studies or evaluations of our water quality management decision-making process so we can begin to complete the information system with a quantitative definition of the "information product" that our monitoring system is to produce.

We really can't begin to complete the system until we fully understand the current state of the art of various components of the system. The program for this symposium has been organized to bring you up to date on the monitoring system, particularly the latter parts of the system--those dealing with the information end.

We begin with Dr. Marshall Moss giving us an overview of water quality data in an information age. Representatives of three different segments of the water quality monitoring field will then respond to Dr. Moss from their perspective.

Next, we have a series of papers that describe efforts toward the design of monitoring systems in different parts of the world. Goals, approaches, implementation strategies, and results can be very different and we can all learn from each others efforts.

We then enter into presentations that focus on more specific topics related to the monitoring system components.

First, we address statistical aspects of monitoring system design--you define an

information goal and then establish your statistics to achieve that goal. Thursday, we move into the question of how do we assure that we have good data to work with? Next, how do we handle the large amounts of data we collect so that it is ready for easy and statistically correct analysis. Data management is evolving rapidly as new computer hardware and software are constantly being introduced. What is happening in the field of data analysis?

While those of us in research often struggle with specific details in our research, many of you have to put everything together and make it work. We finish the Symposium on Friday with a number of case studie where we will learn of the success an failures of people who have had to "get th job done."

We, the organizers of the Symposium, ar very glad you have been able to join us as w discuss this very important topic. Please us the breaks and meal times to visit with eacl other--we all have a lot to learn from eacl other! Please let me know if there i anything I can do to make your time spen here at the Symposium more professionall rewarding or your stay in Fort Collins mor enjoyable.

WATER-QUALITY DATA IN THE INFORMATION AGE

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For those of you who have studied the program of this symposium in sufficient detail, you will note that the two-part initial title of my talk has been truncated. To survey the history of water-quality data collection and make even subjective evaluations of our current level of proficiency in this realm of science, I found to be a task too monumental to undertake in a brief presentation; and to project where we are going without a firm basis of where we now stand would be pure folly on my part. I think that we can congratulate the conveners of this symposium and ourselves if, in the next three days, our deliberations provide a first approximation of where we stand. As to where we are going, each water-quality scientist and program manager will have to make an individual determination, for we are each driven by somewhat different sets of goals and constraints. Although the determinations of where we are going will be individual ones, they are not independent of each other; through the development and implementation of new technology for the generation of water-quality information, a synergistic effect is created that a rational decision maker cannot ignore. My talk this morning will attempt to describe how I think this synergism functions and how we can best take advantage of it as individuals.

The title of this symposium, the Design of Water-Quality Information Systems, is indicative of a significant step in the evolution of the sciences that deal with the quality of the waters of our globe. For too long, we have been concerned with establishment of water-quality data networks without sufficient recognition that the data were not ends unto themselves. Quantification of the information that the data contain and the design of systems that optimize, in some sense, the information that is generated represent significant progress toward rectifying the somewhat myopic views of the past. Yet, information is not an end unto itself either. It has been demonstrated in other facets of water-resources decisionmaking that the economic impacts of data are not linearly related to the information that the data contain (Moss, 1970; Maddock, 1973; Dawdy, 1979). In fact, information that is misused can have a deleterious effect on a decision, and, in such instances, the underlying data can be said to have a negative economic value (Moss and others, 1978).

Samples for chemical compounds that occur at lower and lower harmful at these low levels, new data and information now can be collected for the betterment of humankind. However, for chemicals that do not harm the environment at such concentrations, information on their occurrence in a water body can lead to reactionary and wasteful spending trying to "remediate" a non-problem. Had the data on the existence of the non-harmful chemicals not been available, the hypothetical funds would not be expended. Thus, misuse of the data and their attendant information can lead directly to the worsening of a situation.

The point of the above example is that the design of an information system must be influenced by the decisionmaking technology that will be used in addressing the objective or set of objectives that is the impetus for the system's creation. If the decision technology

and the information system are not coupled at the system-design stage, the impacts of the ultimate decisions almost certainly will not be optimal and may even be negative.

To help clarify how this coupling is manifested, I would like to refer to Figure 1, which is a depiction of an information system and the role it plays in decisionmaking. *Ideally, the information system is imbedded in a natural progression of actions and decisions that begins with the perception of an opportunity and culminates in the implementation of decisions that maximize the net positive impacts provided by the opportunity. Frequently, in the field of water quality, the initial perception is not one of an opportunity, but of a problem. However, by duality, the existence of a problem can be considered an opportunity if some means of minimizing the negative effects of the problem exist.* (We who work in the water resources field would find little opportunity to exercise our skills without the existence of water-resources problems.)

Figure 1 joins the progression at the stage of the conversion of the perceived opportunity into an objective or set of objectives that will be used to direct subsequent decision making. Frequently, the specification of clear, relevant objectives that lead to quantification in the *decision process is one of the most difficult* steps in the progression.

Once the objectives have been chosen, appropriate technologies can be selected to address those objectives. Selection of the decision technology entails: (1) the choice of *the relevant variables and parameters that describe both the water quality and the socio-economic setting of the opportunity;* (2) specification of the means by which the variables will be combined to dictate subsequent actions; and (3) definition of the process for dealing with the inherent uncertainties in the variables and parameters. *With the decision technology firmly in mind, the designer of the information system can* specify the procedures to be used to analyze the water-quality data. These data-analysis technologies may be any one or a combina-

tion of models that account for th probabilistic, stochastic, or determinist natures of the water-quality phenomena c interest.

In the ideal setting depicted in Figure each of the steps described above should b taken prior to consideration of the design c a water-quality data-network. The design c the data network answers the questions: (1 what is to be measured, (2) where is it to b measured, (3) when is it to be measured, an (4) how accurately is it to be measured Network design has been depicted (Moss 1982) in a structural analogy as a pyrami(shown in Figure 2. The base of the triangl(is denoted hydrology, but it is hydrology ir the broad sense, ". .. the science that deal: with the waters of the Earth, their occurrence circulation, and distribution, their chemica and physical properties, and their reaction: with their environment, including thei1 relation to living things" (Federal Council fo1 Science and Technology, 1962). In discussing network design for water quantity, I believe that much of the success of early data networks can be attributed to the fact that understanding of the hydrologic processes is the basis for network design. In comparison with the situation in water quality, however, I believe that, frequently, our successes in network design have come in spite of, not because of, the inclusion of process under-standing.

The second tier of the network-design pyramid consists of three blocks. The block to the right is probability. In my opinion, probability theory is the key to understanding what we don't know about hydrology, includ-ing water quality, and networks can never be truly optimum unless they are based on a quantification of what we don't know as well as what we do know. Resting on probability theory is the set of tools known as statistics. Two tools that are commonly used in network design, sampling theory and correlation and regression analysis, are only representative of the full statistical tool box. Capping statistics is Bayesian analysis, which is simply a formalization for quantifying the uncertainties of tiers below.
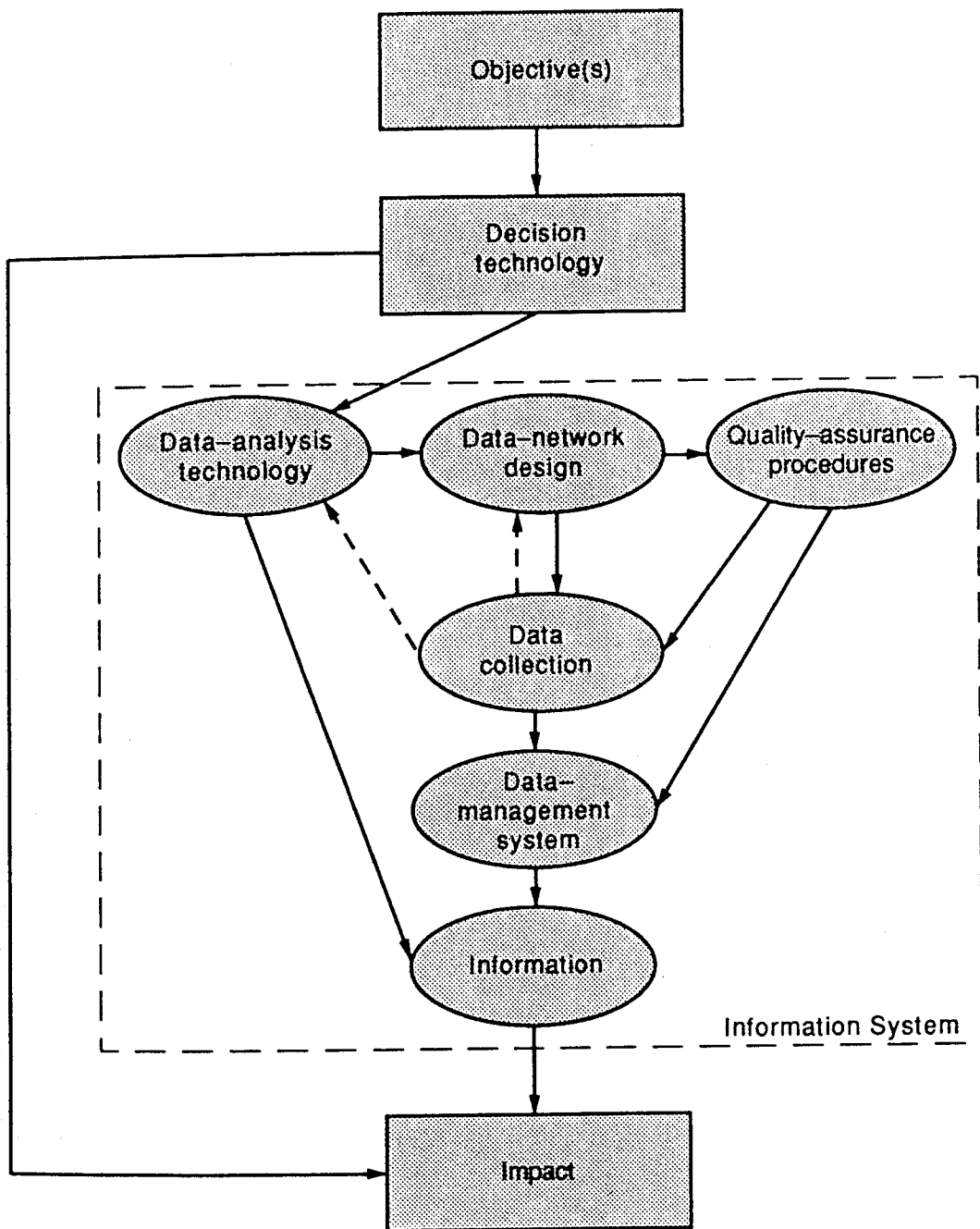
Figure 1--Components of an Information System
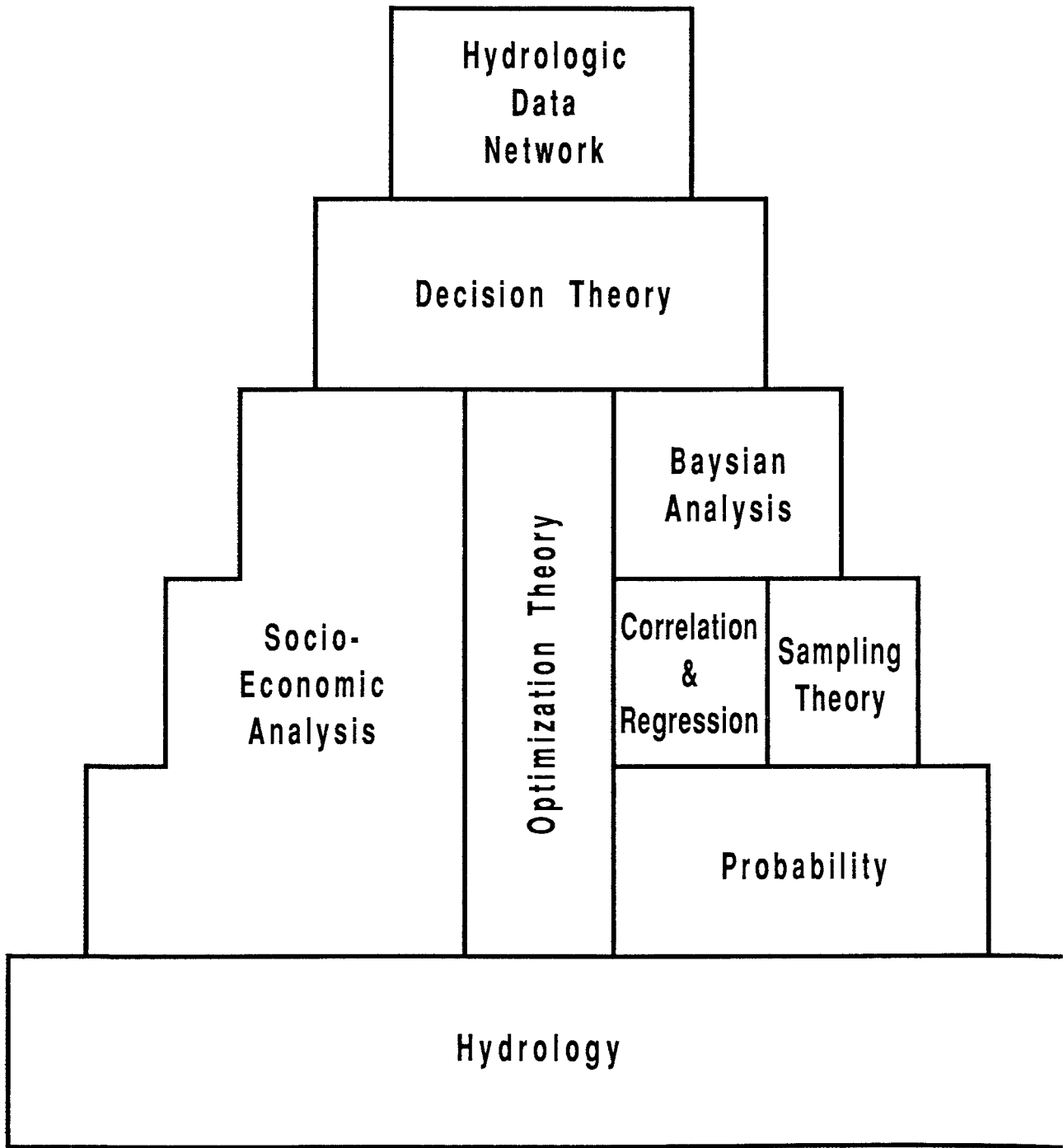
Figure 2--The Basic Building Blocks of Network Design

On the left side of the structure is a somewhat amorphous set of blocks labeled socio-economic analysis, which is not as distinct as the right side because to date we commonly have failed to include it properly in our network designs. I think that these failures can be attributed not only to the difficulties involved, but also to our ineffectiveness in interesting fellow scientists from the fields of policy, sociology, and economics in such problems as they relate to water. However, with respect to the details of the structure, I think that we can hazard a guess that the topmost block also must be Bayesian analysis. Surely, the uncertainties of socio-economic analysis are at least as great as those in hydrologic analysis.

The central pillar of the pyramid is labeled optimization theory and represents another set of tools. Its central location is not due to its relative importance vis-a-vis the blocks to either side, but because of the hybrid nature of many of its components. For instance, optimization is used in defining the parameters of many deterministic models that describe basic hydrologic understanding. Thus, optimization theory is contiguous to the very base of the structure. Similar examples can demonstrate its relevance to each of its adjoining blocks.

The capstone of network design, upon which the data network itself rests, is decision theory. Decision theory is the integrator of all components below it in the structure.

As might be suspected, the real world does not always follow the ideal prescription. For example, consider the National Stream Quality Accounting Network (NASQAN) operated by the U S. Geological Survey. The Geological Survey saw the establishment of NASQAN as an opportunity to redress the set of generic problems with U.S. water-quality-data bases pointed out by Wolman (1971). Those problems were: (1) short record lengths, (2) changes in locations and frequencies of data collection, (3) incompatibility of water-quality-data collection with hydrologic understanding, and (4) lack of knowledge of temporal variability as a prerequisite to detection of significant trends. The objectives

for NASQAN, which evolved directly from the generic problems, were: "... (1) to account for quantity and quality of water moving within and from the United States, (2) to depict areal variability, (3) to detect changes in stream quality, and (4) to lay the groundwork for future assessments of changes in stream quality" (Ficke and Hawkinson, 1975). However, there is no evidence in the published literature that indicates that design of NASQAN took into account the decision technologies nor the data-analysis technologies that would be used to address those objectives. Therefore, the inevitable budgetary pressures have caused NASQAN to be modified without the benefit of knowledge as to how the changes would impact the network objectives. In response to this situation, the Geological Survey is performing a thorough redesign of NASQAN that has begun with revisiting its objectives. In this redesign, data-analysis technology, particularly for trend detection, is playing a major role.

Subsequent to the design of the network, it is possible to take the answers to the "how-accurate" question and develop procedures to assure the potential user that the quality of the water-quality data are known. Traditionally, many data users have been simply too pleased by the existence of a data set to question its accuracy; their attitudes seemed to be that the data may not be perfect but it's the best information available. As more water-resources decision-makers become aware that their decisions are sensitive to the quality of the data that they use, the issue of quality assurance becomes more important. As an extreme example, the expenditures for quality assurance of data collected by the Geological Survey in support of the decisions concerning the Nevada Nuclear Waste Storage Site are of the same order of magnitude as those for the collection of the data themselves.

At this point in the progression, actual data collection can begin, and it is also at this point that feedbacks, represented as dashed arrows in Figure 1, ideally begin to take place. All of the previous steps were based on a specific level of knowledge about the water-quality conditions of interest. As data

are collected, this level of knowledge increases, and new data-analysis techniques and new network designs may be appropriate.

In the information age, no discussion of information systems would be complete without a few words about data-management systems. Part of the synergism mentioned earlier can be attributed to the existence of robust data-management systems, like the STORET system of the U.S Environmental Protection Agency and WATSTORE of the Geological Survey. The information contained in properly identified data entered in such a robust system is available for a multitude of uses other than those for which it may have been originally collected. But, with robustness comes a price tag. The first part of the cost of a robust system is that the options inherent in such a system tend to make it difficult to use; this part of the cost can be minimized by user-friendly system design. The second cost is the potential loss of information that the robustness entails. Because the data-management system cannot be all things for all people, compromises must be made. These compromises usually result in data compaction or loss of data attributes, such as its accuracy and quality--each of which is a diminution of information. To ameliorate the loss of information, subsystems that retain more objective-specific information can be appended to the central, robust system.

The product of the information system is ultimately developed by processing the data through the same data-analysis technology that initially was crucial in defining the data network. The progression culminates by integrating the water-quality information into the decision process for which it was designed to have an optimal impact. The key to obtaining this optimality is the compatibility among the decision technology, the data-analysis technology, and the data network.

Now, I would like to return to the concept of synergism in water-quality information systems. I think that such synergism can derive in three ways. Firstly, information is a commodity that is not destroyed by its use. Thus, if it is properly preserved, it can be made available at minimal cost for many uses

that were not anticipated at the time of its collection. Secondly, information can be used to improve understanding of water-quality processes. By improving process understanding, the information content of the existing data and all future data are enhanced. Thirdly, synergism evolves from our taking advantage of the accomplishments of others. New approaches and new technologies for the design of information systems, like the data they contain, are recyclable commodities.

To illustrate the unrealized potential for synergism in water quality information, I would like to relate some results from a study that the Geological Survey has conducted here in Colorado. This study and a companion conducted in Ohio surveyed Federal, State, local, and regional agencies and universities to determine the amounts and types of water-quality data collected during the 1984 water year and to determine how many of those data could be collated to define the ambient water quality in each State. The studies were implemented in a series of steps (Hren and others, 1987), starting with a compilation of all non-commercial entities that might be collecting such data within each State. Within Colorado, 115 data-collection programs were identified. A survey form, sent to the managers of each program, was used to develop a data base for the remainder of the study. The study then progressed with a series of screens to determine whether the data from a program had utility in defining ambient conditions. Phase 1 of the study used five screening criteria:

1. Do the data represent ambient stream or aquifer conditions, as opposed to wastewater effluent or treated water?

2. Are the data available for public use?

3. Can the sampling sites be readily located?

4. Is quality-assurance documentation available?

5. Are the data in computer files?

The 338,000 samples collected in Colorado during the 1984 water year yielded the results shown in Table 1. After screening for the

Table 1--Water-Quality Data in Colorado

	Surface Water	Ground Water	Total
All Samples	308,120	30,080	338,000
Available/ Ambient Conditions	145,470	12,310	157,780
Meeting All Phase I Criteria	105,840	8,440	114,280

first two criteria, that is, publicly available measures of ambient quality, the number of remaining samples was reduced by more than half. The main factor causing this reduction was the elimination of samples that were collected for the permit requirements that could not be related to ambient conditions. After application of the final three criteria, only about one third of the original samples remained. Of the final three criteria, computerization of the data was ihe most stringent.

The second phase of the study expanded the analysis to investigate the adequacy of the quality-assurance programs (Oblinger, Childress, and others, 1987). The 114,280 samples that passed phase 1 were determined to have had 240,000 analyses and measurements performed on them. The quality assurance of the field and laboratory procedures used to make these analyses and measurements were explored in some detail, and it was found that only 26,400 of the analyses and measurements had adequate quality assurance for the purpose of determining ambient conditions. The major deterrent to data adequacy was the lack of representativeness of the samples collected in the field. If two thirds of the samples were deleted in the first phase and then almost ninety percent of the measurements performed on the remaining one-third were deleted in the second phase, it seems that there is ample opportunity for future development of synergism in Colorado.

I would like to close with a note of caution. If synergism is created by three factors, it also can be prevented by three factors. Lack of adequate quality assurance procedures, both in data collection and in its management, preclude the perpetuation of the data's information. Second, poor access to the data limits its information utilization as well. Lastly, poorly informed managers and users are perhaps the biggest drawback to attaining the desired synergistic effect. The obvious remedy for this last malady is the one that you are all taking by being at this symposium.

Thank you.

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"WHY MONITOR?"

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INTRODUCTION

In his keynote address, Marshall Moss highlights a critical aspect of the monitoring business that appears to be at the heart of our previous successes and failures: clearly articulating goals and objectives that are responsive to the needs of decision makers. These goals and objectives not only drive the design of water quality information systems, but also determine whether long-term monitoring programs can compete for resources with shorter-term research and management activities. Managers often ask, "Why should I spend a dollar on monitoring to find out in five years that I have a problem when, instead, I could use that dollar to fix a problem that I know I have right now?" That is a good question!

Paul Portney of Resources for the Future thinks that, in order to make economic sense, monitoring programs should save at least as much as they cost by targeting control and mitigation resources at the highest-valued outputs. Monitoring goals and objectives thus should be tied to decisions: should enforcement activities focus on one polluter or another; should limited research dollars be applied to acid rain or non-point source pollutants; should expensive control programs be continued unaltered, modified, or abandoned?

My remarks today are based on my experience over the past two years in designing an Environmental Monitoring and Assessment Program (EMAP) for the EPA's Office of Research and Development. The broad goal of this program is to assess the status and trends in the condition of the nation's ecological resources at the regional and national scale. Its objectives are to determine whether the sum total of our environmental protection efforts are truly protecting our ecosystems, and if not, where additional efforts should be targeted.

I also should say that these remarks represent my own point of view and not necessarily those of the EPA. This is not just a disclaimer. EPA's monitoring responsibilities are spread throughout at least a half-dozen offices (EPA 1989), each with their own goals and objectives. Unanimity of opinion would probably be undesirable. I also will make some assertions that are meant to pique your curiosity, but which may not stand up under careful scrutiny. I encourage you to take issue.

MONITORING-- BANDWAGON OR A GOLDEN AGE?

We appear to be entering a period of widespread receptivity toward monitoring in the environmental community in general. Virtually every federal agency has a major initiative for FY 1990 aimed at inventory and monitoring of the resources for which they are responsible. I believe that this phenomenon is being driven by at least three forces in our information-based society: the needs for 1) better information for decision-making, 2) empirical data to confirm or precede complex theoretical models, and 3) demonstration of success.

The incremental cost of solving problems increases exponentially as you near the endpoint, whether it is removing the last ten percent of a pollutant from a waste stream to putting the finishing touches on a final report. We have made considerable progress on the simple, low-cost part of the environmental problem solving curve. Rivers no longer

catch fire, epidemic waterborne disease is a thing of the past, and many previously "dead" lakes again support commercial and game fisheries. Solving the more subtle, long-term environ- mental problems that remain is going to be more costly and will require that we focus our limited resources on the most problems and regions where the current or potential damage is the most serious.

This thinking is the basis for the "risk-based approach" adopted by the EPA to focus its regulatory activities (EPA 1984, Yosie 1987). The concept of prioritizing toxic and carcinogens for regulatory action based on a comparative hazard evaluation which takes into account potency and expected exposure levels is by now familiar to all environmental scientists. This approach is helpful when considering releases of chemicals a priori, but what about retrospective, ecosystem level risk? How many stream miles are unsuitable to support a healthy fish community because of acid rain, versus point and non-point sources of pollutants or habitat loss? How do the percentages vary among regions? With what confidence do we know the answers to these questions? If we had the data, how would they be used to prioritize research funding or regulatory attention? Monitoring information is needed to answer these questions.

Monitoring data also bolsters our confidence when theory is underdeveloped or lacking. Observation of severe or widespread damage often is sufficient to force action, and observational data carry more weight than model results in the decision-making process when confidence in the latter are low. Complex ecological responses to alternative management options are difficult to predict with much confidence. Over the past several years, there has been a tremendous increase in the attention given to several air pollution issues. While a theoretical understanding of the underlying physical processes is an important factor in the current scientific and regulatory thinking, I encourage you to reflect on the relative impact of theory (process studies and modeling) and observation (environmental monitoring data) relative to several of these issues.

Field observation that acid deposition harmed ecosystems and derived from anthropogenic emissions apparently preceded quantitative theoretical understanding of the issue by a century (Cowling 1982). Widespread concern over acid deposition in the U.S. appears to have come about in the mid-1970s with the publication of regional deposition maps and findings of widespread declines of fish populations in acidified Adirondack lakes. Even today, our regional acid deposition models (e.g., Schwartz 1989) appear to be less influential than empirical observations relative to determining acceptable reduction strategies. The observation of the Antarctic ozone "hole" and smaller lower latitude stratospheric losses appear to have precipitated international action (the Montreal Protocol) even though theoretical predictions of the effects of nitrous oxide and CFC's on stratospheric ozone were made over a decade ago (e.g., McClroy and Salawitch 1989). The possible effects of increasing tropospheric carbon dioxide on global warming have been known for decades, but the ability of current general circulation models to quantitatively forecast future regional responses is poor. Recent public concern appears to have been driven more by the observations that 1) tropospheric levels of greenhouse gases have shown dramatic increases over the past decades, and 2) we have had a run of unusually warm years during the past decade (e.g., Kerr 1989).

In addition to stimulating concern and action, monitoring data also often serve as the basis for empirical management models that often precede more complex simulation models based on first principles, as elegantly illustrated by Rigler (1975) for the development of trophic state models for lakes. By analogy, Dawes et al. (1989) recently found that clinical (theoretical) assessments of mortality from most diseases in humans are not significantly superior to actuarial (empirical) assessments.

Finally, the increasing incremental costs of problem solving makes environmental consumers cost-conscious. They are not content to know that something is being done, but

express a right to know whether the current pollution control expenditures of $70-80 billion each year are solving the problem. There have been increasing calls from Congress, scientists, and the public for programs that disseminate environmental statistics to the public that could be used to judge the success of current efforts and the need for new ones (House of Representatives 1985, Portney 1988, GAO 1989).

PROSPECTS FOR EFFECTIVE GOAL-SETTING

Given that the current scientific, managerial, and public climate appear to be right for the inception of new monitoring efforts, what are the most likely roads to success? What are the most likely pitfalls? How are they related to the goal-setting process?

A workshop was held at Cary Arboretum several years ago (Strayer et al. 1986) to identify the critical components of successful long-term monitoring programs. The attendee list read like a "Who's Who" in long-term environmental research. The participants concluded that the most critical elements in successful programs were: the commitment of a "champion" who guided and defended the program and provided continuity and cohesion; clearly articulated goals and objectives; and a vigorous program in analysis, interpretation, and reporting of the data. How do these criteria compare to the typical situation in monitoring programs?

Interviews with federal monitoring program managers during the EMAP planning process revealed that programs tended to come and go as influential champions in the bureaucracy came and went, that goals and objectives were usually too broad to provide a clear measure of likely or actual success, and that the first item to be sacrificed under the budget ax was data analysis. Lack of a single "champion" has not spelled doom, however, for such a long term "monitoring" programs like the Census, various labor statistics, the Dow-Jones Industrial Average, or the nation's meteorological and hydrological monitoring programs. Each of these programs does,

however, produce high quality, interpretive data products that form the basis for a great deal of planning and decision-making. Imagine life without these programs! While they undoubtedly have produced benefits and met needs not articulated by their originators, their central utility in decision-making is clear.

Let us assume for the moment that insuring the commitment of a champion is either beyond our control, or may be critical only up to the point that the program is producing decision-making products that are of undisputed value. We also must accept that, however valuable the data might be, a monitoring program will fail if they are not communicated to decision-makers (including the public). Given these points, how can goals and objectives be used to maximize the success of a new program?

The most common problem in goal setting is lack of specificity. At the broadest scale, this results in "motherhood" objectives that provide little guidance to the design of the information systems that are the topic of this symposium. As an example, the broad goals and objectives of the U.S. Geological Survey National Water Quality Assessment Program (Hirsch et al., 1988) and those of EMAP are virtually identical. Discussions between USGS and EPA scientists and planners, however, revealed that the programs are complementary, in neither case were the stated goals and objectives sufficiently precise to unambiguously define the information needs.

Lack of specificity often arises from trying to summarize a complex idea in a few simple "bullets" for a briefing or executive summary. Occasionally, specificity is seen as restrictive and is avoided to keep from foreclosing options, and objectives tend to evolve with the policy climate surrounding a management issue.

Several technical issues appear, however, with alarming regularity; one is that of scale specification. Acute problems occur over short time scales and affect local resources and individuals or small groups. Chronic problems occur over several years to decades and affect regional resources and populations

of individuals. Goals and objectives of monitoring programs vary with these scales. In a zero-sum game, tradeoffs between temporal and spatial coverage may require different monitoring designs for the two types of programs. Local jurisdictions need programs that monitor sources and receiving media at relatively high frequencies to target local and site specific problems. Regional and national jurisdictions may conduct broad surveys at annual or semi-annual intervals to assess the need for changes in regional and national strategies.

As an example compliance monitoring programs may be targeted at single polluters (e.g., NPDES permits) or at multiple polluters in some jurisdiction (e.g., attainment of ambient air quality in metropolitan areas). Compliance monitoring tends to set very specific targets on effluents or ambient medium quality very near the source. This approach maximizes enforceability, but does not confirm that we are protecting complex ecological communities in receiving streams or the health of people exposed to air pollutants in their homes, offices, and auto-mobiles. Furthermore, the programs could be under- or over-protective. Violation of dis-charge standards could result in occasional fish kills that do not affect long-term community structure in streams, and humans may physiologically adapt to air pollutant concentrations that violate primary standards. On the other hand, unknown pollutants, synergistic effects, or other problems may limit attainment of ecosystem quality or public health goals. Monitoring ecological communities and environmental epidemiolog-ical data answer these questions, but are usually very difficult to link to enforceable actions.

Other technical issues have to do with applicability of seemingly "generic" monitoring information. In the water quality area, for example, there is a cherished tradition that water bodies integrate the goings-on in their watershed (Hynes 1975). Spatially complex processes in soils and disparate vegetation types thus are integrated at some point in a lake or stream and can be monitored on a scale ranging from hours to decades. From a management standpoint, the integrative nature

of sampling points is relevant and appropriate to the quality of water withdrawals Conversely, if habitat is the issue, it is no the average water quality at some downstream node in a watershed, but the distribution o water quality throughout the reaches in the watershed that determines the overal condition of the system. Anyone who has tried to balance an element budget for a lake based on routine monitoring data also appreciates the difference between a program aimed at collecting monthly grab samples to estimate average water quality conditions and one designed to estimate loadings.

The National Acid Deposition Program National Trends Network (NADP/NTN program was designed to measure acid deposi tion rates, based on a large number of fixed site monitors. Time series of data can be analyzed to determine whether deposition rates are increasing or decreasing at one site or at groups of sites. This is not quite the same, however, as answering the question "What is the average mass input of sulfur o nitrogen to the region where the collectors are located?" Dry deposition is not accounted for, and the collectors have been sited to avoid "local" pollutant sources and poorly represent higher elevations possibly coasta locations. Locations that have been excluded to avoid "atypical" data that interfere with trend analyses that the networks were designed to measure are certainly part of the ecological regions in which they are located and may contain some of the most sensitive ecosystems.

Increasingly, it appears that programs tha are well-designed to meet one set of goals and objectives are of less utility when applied to new goals and objectives. The issue is less often data quality than data applicability Scott Overton of Oregon State University also points out that, like money buried in a shoe box, the value of data depreciates with changes in analytical techniques and our level of understanding of ecosystem processes and effects. You are all aware of problems with early analyses of alkalinity, phosphorus, heavy metals, and plankton and microbial counts a a basis for comparisons with current condi tions. This is not to say that "found" data and networks cannot provide valuable

information when used in new contexts, but it may be overly optimistic to expect them to fully meet new goals and objectives.

ANALOGIES AND ATTITUDES

I have become increasingly interested in analogies related to environmental monitoring as a way to explore issues relating to scale, applicability, and value of monitoring systems. For the new golden age of monitoring to last more than several years, I think that our ability to analogize may be critical to our success in implementing and maintaining monitoring programs. Two analogies appear to me to have the most to offer: corporate practice and the health field.

There is a school of thought that government agencies are simply businesses that are unusual in the way that they handle information (Weisbrod 1989). If this is the case, then those of us in the environmental business provide environmental technology and regulation products and services to the consumer. Just as in a business, we are constrained and protected by certain rules and laws. The analogies to monitoring in business appear to be market surveys ("anticipatory monitoring"), quality assurance (compliance monitoring), and sales figures and consumer surveys ("effectiveness monitoring"). Anticipatory monitoring programs seek to discover the extent and magnitude of emerging problems as a way to target resources at the most needed environmental products. Public opinion plays a critical role in this process, but objective scientific data are needed to inform public opinion. Compliance monitoring determines that our products and services are as we designed them to be. Finally, effectiveness monitoring programs determine that the product, however well made, is providing a service (i.e., environmental protection and improvement) valued by the consumer. Again, technical surveys assure that the consumer is accurately informed.

Imagine a food company that responds to every idea in the suggestion box for a new cereal or ice cream flavor or a book company that publishes a 2000-copy run of every manuscript that is submitted. On the contrary, only a small fraction of products receive the marketing and promotional attention needed to establish a successful product. Imagine an automobile company that continued to market the Edsel despite lackluster sales, or a television network that continued to broadcast a program with a small and diminishing viewer share. Corporations spend vast sums on monitoring to trumpet successes and to limit their losses on mistakes. Would this not appear to also apply to resource management agencies at all levels of government?

One reason for the luke-warm reception given to "anticipatory" or "effectiveness" monitoring is our awareness of our limited understanding of the environment. We are concerned that our tools are too primitive to deliver the promised product, or that there are too many problems confronting us at once. It is here that I find the medical analogy helpful. Very few physicians are blamed for not saving their patients from lung cancer. On the other hand, we need to know how best to allocate research resources among lung cancer, heart disease, AIDs and other diseases to minimize the overall risk of premature death from some disease. Society also has a right to expect that unsuccessful programs to reduce risk will give way to more successful approaches.

Who stands to win and lose in such a scenario? Aggressive monitoring in the corporate world provides products and services that best meet consumer needs. It seems reasonable that the same would be true for government. The careers of individuals responsible for introducing new products or services stand to suffer if their projects cannot create a new market or compete successfully for current market share. These individuals thus are usually insulated from the monitoring process, which often is conducted by outside "survey" organizations in the corporate world. If the analogy is reasonable, monitoring programs other than quality assurance (compliance) in government agencies might best be isolated internally from the line organization responsible for development and implementation of regulatory programs.

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CONCLUSION

I have tried to make a case for the difficulty and importance of specifying the goals and objectives that drive monitoring design. Designers of water quality information systems must seek specific goals and objectives from decision makers that are sufficient to allow them to present example expected outputs to the decision-makers and to ask them whether these outputs are necessary and sufficient to make such decisions. Designers should be aware of the alternative uses of the data, as outlined above, and determine what kind of program is envisioned, being especially aware that there are likely to be conflicting viewpoints as to what monitoring should accomplish, Designers must be on the lookout for differences in scale, purpose, or applicability that may make competing programs complementary, rather than duplicative. Finally, designers should be prepared to interact continuously and proactively with decision-makers to make sure that the resulting data will reduce, rather than increase, the overall cost of environmental protection.

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WATER QUALITY INFORMATION SYSTEMS: PAST, PRESENT & FUTURE AN INDUSTRIAL PERSPECTIVE

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INTRODUCTION

The design of water quality information systems plays a key role in industry's environmental monitoring programs. This paper presents a brief chronology of the evolution of one such program, the present state of the art and some thoughts on future challenges. The paper centers on an outline of the information flow of a monitoring program as described by Sanders et al. (1983).

Central to the theme of the symposium is the distinction between "data" and "information." Data is a basic set of numbers collected with some purpose in mind. The data, however, may be collected without a preconceived, specific statistical objective. Little or no thought may have been given to the errors associated with the data gathering process. The ultimate impact of these errors will be to lower the information content of the data. Decisions based on the results of the monitoring effort may be erroneous.

Information, on the other hand, is a set of numbers gathered with a group of specific objectives in mind for which the data will be analyzed and used. The transformation of data into information requires that we know why we have collected the data, how we intend to use the numbers (statistically analyze and report the data) and that we have a basic understanding of the uncertainties associated with the data. It has been pointed out (Rogers 1982) the most important factor associated with reporting data is a clear statement of the uncertainties which are a result of the environmental matrix from which the data is collected, the sampling and the analytical process.

This symposium represents efforts to describe a water quality information system based on the transformation of collected data into useful information.

PAST

Industrial experience with a groundwater monitoring program can be viewed as a ten year evolutionary process (Figure 1). The process began with the mere collection of data and now focuses on the information product of the system.

The program was characterized by the collection of large numbers of groundwater samples, the analysis of those samples, and some rudimentary attempts at data analysis. The goals were simply expressed and were meant to describe the groundwater quality at an industrial site by answering the following questions:

Does contamination exist in the groundwater?

Where in the aquifers are the contaminants located?

What are the sources of the contaminants?

Are the contaminant concentration levels changing?

The early programs collected large amounts of data containing very large amounts of variability. Attempts to statistically analyze the data were usually unsuccessful. Although large amounts of data were collected, the ability to turn it into information was severely limited (Figure 2).
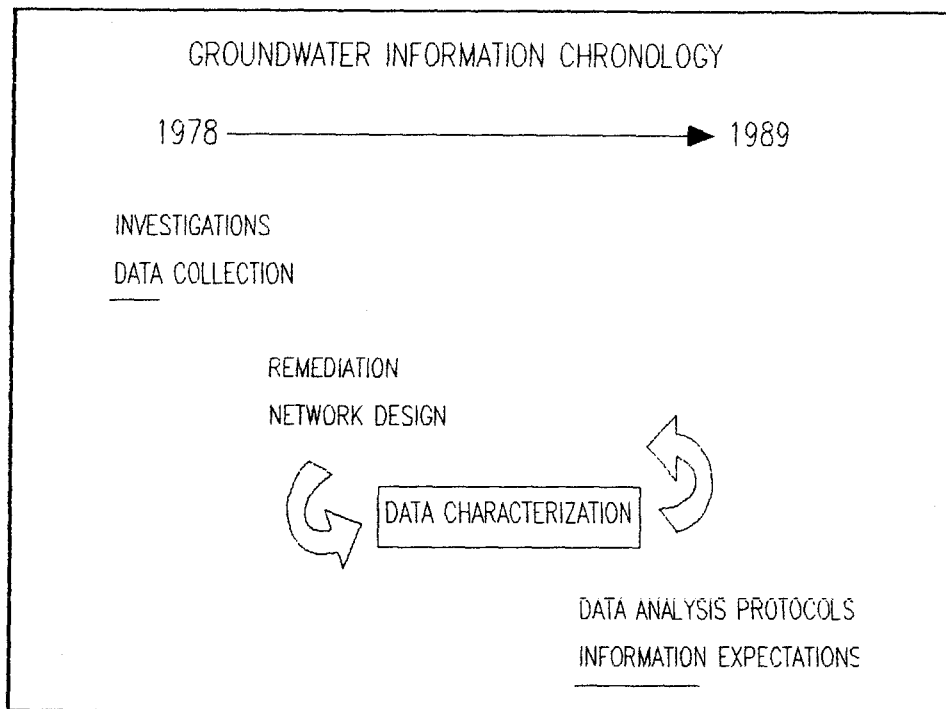
Figure 1.

Figure 2.

Ward et al. (1986) have referred to this as the "data-rich, information-poor syndrome".

There were techniques (monitoring network design, Figure 3) available which made use of data and common statistical procedures and presented a more systematic approach to data collection and interpretation. These concepts offered a uniform approach to the choice of sampling locations, frequencies and statistical analysis procedures.

These methodologies began to stress the need to better define the information goals of the monitoring program prior to data collection.

The implementation of monitoring network design concepts resulted in reduced data variability. This was a primary result of the quality assurance programs which were begun during this time period. Key components of the program are the implementation of uniform sampling frequencies, sample validation procedures (which prevents data containing gross errors from entering the data base), and a more uniform approach to data analysis.

If the overall variability of the data was to be reduced and satisfactory statistical techniques for data interpretation were to be implemented, then additional factors ("data characteristics") had to be taken into account. Traditional statistical procedures frequently failed when applied to environmental data sets because the data sets were small and usually were not normally distributed. In addition, other "data characteristics" such as seasonality, correlation, missing data, censored data (nondetects), trends and variability resulted in data sets which require a careful choice of sample collection patterns and statistical methodologies.

PRESENT

Past experience proved that it was necessary to develop protocols (Ward et al. 1988) to guide the data analysis procedures (Figure 4) and to help deal with the characteristics commonly associated with environmental data.

This would enable "non-statisticians" to work with the data, make auditable decisions and provide a consistent approach. This approach is less subjective and does not vary with personnel changes.

During this time frame, the concept of a set of "information expectations" (Figure 5) was advanced by Ward and McBride (1986). These guidelines delineate the steps leading from a reason to monitor (management and monitoring objectives), to how the data are analyzed and reported.

This approach is auditable, consistent and transferable to new management and personnel if required. Defining information expectations should be the first step in any monitoring program.

The core of a water quality information system is a combination of a set of information expectations, a data analysis protocol, a quality assurance program and a data base management system. The absolute

importance of these key items and the need to implement them before the first sample is taken, cannot be overstated. Consideration of any other approach will likely lead to the data rich, information poor syndrome discussed earlier.

FUTURE

What are additional factors to consider based on past experience in establishing a water quality information system? There are three items:

1. Visual interpretation of data.

2. The role of the legal community in the development of information systems.

3. The education of peers in the concepts of water quality information systems.

Based on experience, it is abundantly clear that in many cases, environmental data sets are of such small size and high variability that the sole reliance on statistical data analysis procedures leaves much to be desired. The use of visual (graphic) methods of data

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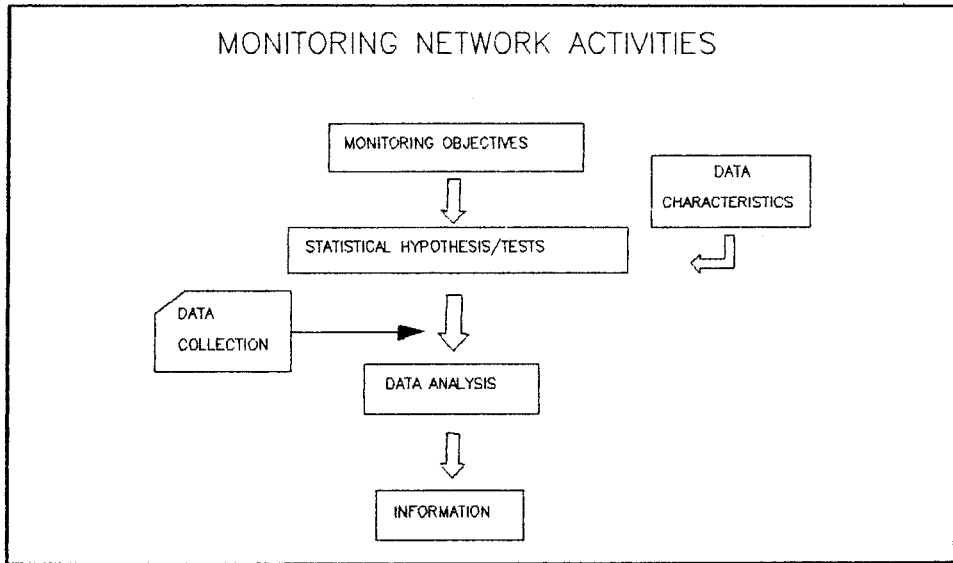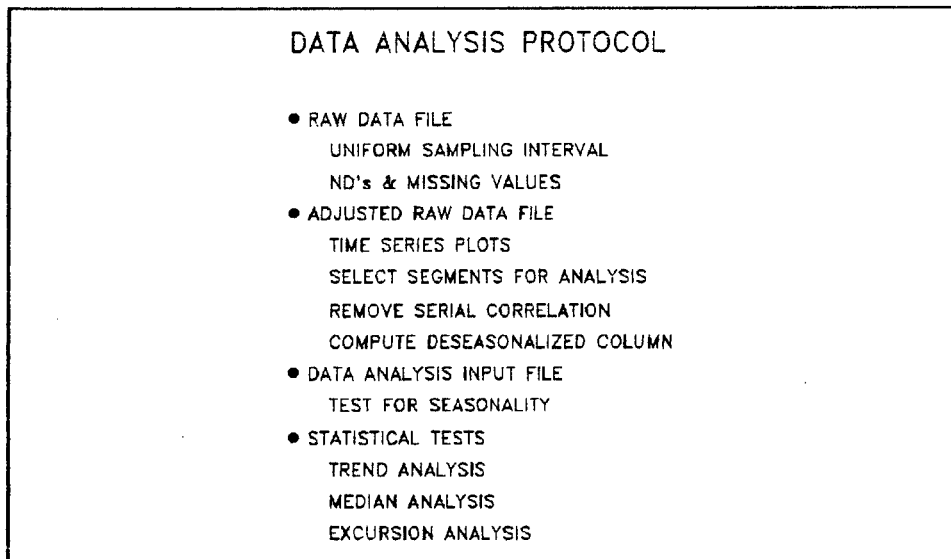
Figure 3.

Figure 4.

INFORMATION EXPECTATIONS

- MANAGEMENT GOALS
- MONITORING GOALS
- DEFINITION OF WATER QUALITY
- STATISTICAL
  - METHODOLOGY
  - HYPOTHESIS
- MONITORING SYSTEM PRODUCT
- REPORTING

Figure 5.

interpretation often provides insights into the information contained in a data set and possibly can suggest alternative (objective) statistical procedures. For example, seasonality in small data sets can often be detected visually (and accounted for when interpreting the data) long before statistical techniques are capable of confirming the cyclic pattern. The majority of the data analysis protocol mentioned above is merely a way to set up uniform and consistent data files and carry out visual interpretation of the data prior to the choice of appropriate statistical procedures. This turns the data into useful information. The excellent books by Chambers et al. (1983) and Tufte (1983) should be required reading for all who plan to develop water quality information systems.

A key item not discussed previously nor explicitly mentioned as a topic for the Design of Water Quality Information Systems Symposium is the role of the legal community in the information process. Many management and monitoring goals are the direct consequence of a legal decision (regulations) such as water quality standards. In the United Sates, standards are considered absolute numbers. The true risk associated with the violation of a standard as well as all the uncertainties related to the measurement processes are seldom considered in either the development of a standard or its application in the monitoring program. Very little information exists with respect to the true health risks of contaminants in the environment. Therefore goals for standards are set at "zero" concentration levels and working standards (such as maximum contaminant levels, MCL's) are defined by the present state of the art of our analytical instrumentation. This process has been termed "regulation by analytical chemistry" by Dowd (1985). One can expect that analytical sensitivities will continue to increase. The potential impact on monitoring and remedial action resources must be considered. These resources are not infinite, therefore they must be carefully allocated on the basis of objective priorities.

There is a rising awareness in the legal community to the uncertainties associated with data collection and information processes

(Ng 1989, Koorse 1989). Informatio managers must take a more active role i educating the legal community in an attemp to more adequately control the allocation of environmental resources through the prope use of informa- tion systems. At the sam time, we must try to understand the legal pro cess and the liabilities that the collection of data might entail.

Last, but not least, we must address th question of the education of our peers. Th breadth of topics to be discussed at the De sign of Water Quality Information System Symposium indicates a wide range of interes in the concepts of the information processe: There is clearly tremendous interest in th subject and a desire to apply the principle gathered by plan and circumstance in a effort to more efficiently carry out the tasks

Unfortunately the necessity to develoj information expectations and data analysi protocols is not always apparent to all wh must begin to collect or are collectin, environmental data. In many cases the nee to develop an information system is viewed a just one more bureaucratic step, somethin, which results in increased costs and tim delays for a monitoring program with littl apparent value. Data users seldom realiz that there is a problem until they are wel into the data gathering process and attemp to analyze the data. At this point, the dat may not be amenable to analysis and valuabl time and resources may be lost.

The goal for information managers is t clearly explain the necessity of water qualit information systems. The concepts o information expectations, data analysi protocols, quality assurance and databas management must be defined. We mus convince our peers that the time an resources committed to the development of ar information management system will show a return on investment in the long term. I must also be made clear that ignoring these concepts may result in the misinterpretatior of data and incorrect actions based on false assumptions.

The challenge is to clearly show the difference between "data" and "information,'

provide the information systems which efficiently collect and process data and to strive to make the concept of the information system the first item in any monitoring program.

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THE EVOLUTION OF A WATER UTILITY'S WATER QUALITY INFORMATION SYSTEM

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INTRODUCTION

The water supply system for the city of Portland, Oregon, is comprised of a 106 square mile protected watershed, a 22-well groundwater system, and a distribution system, serving a population of approximately 700,000. Sporadic collection of data on the system's water quality has taken place over the last 100 years, but systematic development of a true water quality monitoring network and information system has been limited to the past twenty years. In that time, a sampling network and a data management system have been developed, and a process of using the data to inform users of any significant changes in the network (which hopefully represents the system being monitored) has evolved. This evolutionary process is a cyclic one of collecting data, extracting information from it, acting on that information by changing something and/or collecting new data, and repeating the cycle in a series of iterations.

What is now becoming clear, though, is that the quantity and quality of data being amassed should produce answers to questions about the functioning of basic processes: "How does the system work?" Only recently has the monitoring system, and the Water Bureau's use of the system, matured to the point of being able to suggest, and perhaps answer, process-oriented questions about the quality of water in the supply system. The next step in the development of the water quality information system, it is felt, is to formulate these types of questions on a regular basis in the operation of our data management system. This paper will describe the existing water quality information system used by the Portland Water Bureau, showing how it evolved from its beginnings as a simple data-collection network. Some examples of process-oriented questions will then be given, and the direction that the answers to these questions suggest to future development of the information system will then be discussed.

SYSTEM BEING MONITORED

The city of Portland is located in northwestern Oregon, at the confluence of the Willamette and Columbia Rivers. The population of the city proper is approximately 430,000, but the entire metropolitan area contains about 1,000,000 people. The Portland Water Bureau serves a population of 700,000, either directly or through wholesale purchasers, within a 225 mi^2 (585 km^2) area. Base water consumption is about 105 million gallons per day (MGD) (433 ML/day), while peak summer demands reach as much as 250 to 275 MGD (1030 - 1133 ML/day).

The primary source of water for the system is the 106 mi^2 (276 km^2) watershed of the Bull Run River, located on the western slopes of the Cascade Mountains, about 30 miles (48 km) east of the city. Most of the land in the watershed (about 95%) is federally-owned and is administered by the USDA Forest Service, in consultation and coordination with the City of Portland. The watershed is unique in that it is administered under a federal law, PL 95-200, which pertains specifically to the management of the Bull Run Watershed.

The law provides that the watershed shall be managed principally as a source of "...pure clear raw potable water..." for the City of Portland, and mandates the establishment of

water quality standards, based on historical data, as a means of determining whether the quality or quantity of water produced has been adversely impacted by management practices.

The annual average discharge of the Bull Run River is 530 MGD (2184 ML/day), but low flows in summer can be as little as 40 MGD (165 ML/day). There are two man-made reservoirs and a natural lake with enhanced storage within the watershed, with a combined storage of 21 billion gallons (86,500 ML), that allow demands to be met when they exceed the river's discharge. The intake to the distribution system is located at the dam impounding the lowermost reservoir. The water is coarsely screened as it enters the supply conduits, and is disinfected by application of chloramine, but is not otherwise treated.

Portland's secondary source of water supply is a 22-well groundwater system encompassing six aquifers, located within the city limits along the south shore of the Columbia River. The system was designed for use as a backup supply for the watershed should storage be severelyy diminished or depleted, water transmission from the watershed be interrupted, or water quality problems arise. The groundwater system is capable of pumping 105 MGD (433 ML/day). It has been used to supplement watershed supplies on two occasions, once for three weeks and once for two months, since its completion in 1984. It is anticipated that the groundwater supply will be used more frequently in the future as the population served by the system grows.

Water from these sources is routed through a distribution system that serves a population of 430,000 in a 130 mi^2 (340 km^2) area, with connections to wholesale water purveyors that cover an additional 95 mi^2 (250 km^2) and serve 270,000 more people. The 190 square mile direct service area is divided among seven major pressure zones and contains approximately 1700 miles (2700 km) of distribution mains, connecting six storage reservoirs and 68 tanks to about 150,000 services. Water is brought to the distribution system from the watershed

through three 25-mile (40 km) long conduits, and from the wellfield through a single two-mile (3.2 km) long connector.

SAMPLING NETWORK

Watershed Sampling

The most extensive water quality monitoring in Portland's water supply system is concentrated in the Bull Run Watershed. This concentration of effort results from a number of factors--technical, legal, and political. The technical reasons are the need to address the concerns of source protection for an unfiltered surface supply, the need to assess the effects of land management practices on water quality, the fact that it is the primary source of supply (the groundwater source is used infrequently), and the need to understand watershed processes in order to better manage the resource. Legal factors include the mandate of PL 95-200, which requires that water quality standards be established and used for comparison to current water quality measurements, and regulatory considerations, such as the desire to remain an unfiltered system under the proposed Surface Water Treatment Rule. The political factor that encourages the establishment (and funding) of a large monitoring system is the existence of a strong and vocal public concern over the quality of their drinking water and the potential effects of watershed land use on that quality.

The sampling network in the watershed, as it is currently constituted, uses a three-tiered approach. The first level consists of five Key Stations: four on the major tributaries to the reservoirs and one at the inlet to the distribution system. Water quality standards for 37 different water quality variables, based on historical measurements, apply at each of these stations (USDA Forest Service, 1984a). The second level consists of ten stations located upstream from the Key Stations at the confluences of major tributaries, and four reservoir stations (two on each of the artificial impoundments). The third level in the network is a series of stations in close proximity to the sites of specific land management activities at various locations in the watershed. (USDA Forest Service, 1984b)

The frequency of measurement at the Key Stations--a function of the amount and frequency of collection of data in the historic data base--varies from daily to annually, depending on the location and the constituent being measured. When a particular constituent is found to be outside the range prescribed by the appropriate standard, data from the second and third tiers of sampling are consulted in an attempt to locate the source of the deviation and to determine if any specific land management activity is the cause.

Groundwater Sampling

Because the groundwater system is used infrequently, sampling of the wells' outputs is also less frequent. Except when operating the system as a supplemental supply, groundwater samples are taken when the pumps are exercised periodically (the target frequency is three times per year). During periods of operation for production, sampling is driven by the operating scenario being used. Monitoring concentrates on, but is not limited to, constituents regulated under the Safe Drinking Water Act. Monitoring not associated with regulatory compliance has been conducted in relation to known or suspected sites of potential contamination, such as locations where pesticides or volatile organic compounds have been used, or where iron and manganese levels have the potential to cause problems.

Groundwater monitoring may also be conducted in anticipation of upcoming regulatory action, such as for radon or pesticides. Somewhat greater effort is being put into development of a model to describe the behavior of the groundwater supply. This work, using data from test wells to develop a physically-based model of groundwater movement in the Columbia South Shore aquifers, is being conducted by the U.S. Geological Survey under a cooperative funding agreement with the City of Portland. The project began in 1987 and is scheduled to be concluded at the end of 1991.

Distribution System Sampling

Routine bacteriological sampling of th distribution system was probably the earlies systematic monitoring conducted on any pai of Portland's water supply system. Th current monitoring scheme utilizes about fift sampling points, yielding approximately 50 samples per month, located to sample al supply conduits, in-town reservoirs, and tank: and to give representative samples from th far ends of the major pressure zones. Whil the majority of the samples collected continue to be for bacteriological determinations, majo nodes of the system are also checked fre quently (several times per week to daily) fo chloramine speciation, physical constituents and biological nutrients. Three times per yea distribution system levels of trihalomethan species, metals, and all primary and secondar EPA-regulated constituents are checked.

In addition to routine, scheduled samplin of the distribution system, samples are col lected in response to concerns or complaint: from water consumers. These samples are usually analyzed for their physical and bacteriological characteristics, and occasionally for some metals. Customer response sample: commonly number from twenty to fifty samples per month.

The third type of distribution system sampling conducted involves the establishment of special studies designed to increase understanding of the processes operating within the distribution system, or to give a clearer understanding of the meaning of the routine sampling being conducted. An example of this is a recent study of first-draw samples from domestic plumbing systems that examined the effects of materials and age of plumbing, standing time, and sample volume on the lead concentrations measured. (Lampi, 1988).

EVOLUTION OF THE WATER QUALITY INFORMATION SYSTEM

The Portland Water Bureau's experience in gathering, analyzing, and responding to water

quality information has been that it is an evolutionary process. When presented with an existing water supply system, and asked to answer the question, "What is the quality of the water?" The response is to gather some data and analyze it. When there are no data to start with, the initial round of data collection will necessarily focus on generalities. After studying the information provided by the sampling data, more specific plans for investigating the situation can be formulated.

For example, consider the case where Portland annexed an area served by a small private water system and acquired that system's wells. Initial sampling, just to see what exactly it was that had been acquired, turned up the presence of some synthetic organic compounds. The question then became, "Where did these compounds come from?" The next round of data collection involved study of land use information in the area. This disclosed the presence of certain industrial uses, which in turn provided information on probable quantities and other types of compounds likely to be found at the site. From this, plans for response to the situation (whether and how to treat the water, or to abandon the source) can be formulated.

The development of the Portland Water Bureau's water quality information system has followed such an evolutionary, iterative process. A description of the system's development in three areas--data management, remote sensing, and data analysis and reporting--will show how this process works in somewhat more complexity than the above illustration.

Data Management

Prior to the acquisition of computer technology, water quality data management was limited primarily to simple record-keeping functions. Data analysis was limited to comparisons of observed values with a threshold value or range, usually empirically derived, above or outside of which a problem was considered to exist. No analyses of trends, relationships between variables, or spatial comparisons were performed. Formal reports were generally limited to those required for regulatory compliance, or in response to some unusual event.

The initial impetus toward acquiring a computerized data management ability was given by the development of the watershed water quality standards mandated by PL 95-200. The calculations involved in standards development required that extensive statistical analyses be conducted on fairly large data sets; the work would not have been feasible without the use of electronic data processing. To accomplish this, it was necessary to load the historic data into the computer, which was then used to conduct the initial development of the standards. After the standards were developed, the amount of work required to enter the mass of historic data suggested that new data, as they were generated by the City's laboratory, should continue to be entered into the City's computer data base, rather than let another backlog accumulate. This data base, however, was not used in checking compliance of the new data with the standards, as administration of the standards is the responsibility of the Forest Service.[1] The knowledge and technology of data communications available to these agencies at this time (1984) did not permit this data to be shared electronically. Instead, copies of laboratory data sheets were manually entered into the database, by both of the agencies independently, on a weekly basis.

It soon became apparent that manual entry of the data from the written laboratory sheets had some drawbacks. The additional step slowed the availability of the data for interpretive analysis, introduced an additional opportunity for transcription errors to be made, and did not take advantage of any of the computer's capability for data validation.

[1] Standards development was a cooperative undertaking between the Portland Water Bureau and the USDA Forest Service; the law mandating the standard's development assigned administrative responsibility to the federal agency, but the City of Portland had both a strong interest in the process and better local computing facilities on which to perform the work.

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The next step in the data system's develop-
ment, then, involved the addition of appro-
priate hardware at the laboratory and the
development of front-end menus to allow data
entry by the laboratory analysts directly from
their bench sheets. The data thus become
available for use much sooner, and errors are
reduced by the reduction of the number of
transcriptions and the automatic flagging of
out-of-normal-range values upon entry. The
data are also required to be reviewed and
released by the laboratory director before
being added to the permanent data base.
After this process was implemented, electronic
transfer of data from the City to the Forest
Service was implemented, completely
eliminating the need for hard copy data
transfer.

At this point, the data management system
was being developed to conform to procedures
already established for sample and data track-
ing in the laboratory. As more understanding
was gained of the computer's capabilities,
modification of these procedures along with
further changes in the data entry functions
made the whole process more efficient and
less prone to error, and provided the
foundation for the development of a
laboratory information management system
(LIMS). The system is now being set up to
allow entry of field sample collection data
into the data base at the time the sample is
delivered to the laboratory, and no longer
requires that all analyses for a sample be
completed before the results are entered.
Samples will be tracked by a laboratory
sample number, and thus analyzed as blind
samples, rather than being identified by
station number and time of collection.
Quality assurance and quality control
(QA/QC) functions will also be incorporated,
with these samples (blanks and spikes)
included as blind samples in the sample
stream and the results automatically
incorporated into control charts as they are
entered.

The next step at the data entry end of the
information system will be to develop the
interfaces that will allow the direct transfer of
data from analytical instruments to the data
base. This capability will eliminate
transcription errors (the analyst simply accepts

or rejects the results of a test) and will sav
time and reduce tedium. There are also plar
to procede further in the development of
LIMS, including such functions as samp.
tracking, scheduling, and other functions tha
will be included as the need for them
perceived.

Remote Sensing

Another area in which the monitorin
program is expanding is that of remot
sensing and telemetry. To a large extent, thi
has come about as a result of increases i
understanding of the system gained throug
earlier monitoring programs, which helped t
further define the information needs, couple
with growth in the technology enabling suc
monitoring to be done.

The development of remote sensing as
component of Portland's watershed monitorin
program serves as a good example. Th
watershed monitoring program, as it i
currently constituted, has been carried out fo
about five years. The intent of the progran
was to determine link ages, if any, betweel
changes in water quality at the reservoi
tributaries and land management practices ii
various locations around the watershed. Thi
was to be accomplished through a three-tiered
hierarchy of sampling points (described abov
and in USDA Forest Service, 1984b) wher
regularly-scheduled grab samples are collected
Data collected for development of the stan
dards, and in the early years of their applica
tion, indicated that most of the major impact
on water quality occur during storm flow
(Rinella, 1987), and that periodic grab sam
ples do not adequately represent these effects

In an attempt to remedy this problem, a
storm-sampling program was instituted. A
preponderance of stations and a shortage o
personnel, however, limited this program to a
single grab sample per storm at each station
The data generated from these exercises very
quickly made it clear that this sampling
protocol was inadequate to characterize the
behavior of the system. At the same time, it
was found that the intermediate tier o
sampling stations provided little useful data
to tie together the other two tiers of the
system.

As a result of these findings, planning is now underway to revise the watershed monitoring system. The second tier of stations will be reduced or eliminated, allowing reallocation of some of the monitoring resources. The thrust of this reallocation will be first toward developing continuous automated monitoring (including remote telemetry and automatic sample collection) at the reservoir tributaries, and second toward conducting research that will provide a better understanding of natural and anthropogenic processes occurring in the watershed.

Experience with remote sensing in the watershed has led to an appreciation and awareness of its capabilities. As a result, at the same time that these data collection systems are under development in the watershed monitoring program, opportunities for similar applications are being identified in other parts of the system. This has led to potential links between remote sensing and the information technology that is being planned for water supply and distribution control purposes. Systems are now being implemented for the remote monitoring and control of supply functions such as system pressure, pump status, and tank levels. These systems, with the addition of the appropriate transducers, can also measure and record water quality constituents of interest throughout the water system.

Data Analysis and Reporting

As was indicated earlier, the initial development of Portland's water quality monitoring system concentrated almost exclusively on data collection with very little effort spent on analysis and reporting of the information contained therein. One of the first steps toward routine data analysis came with the requirement for development of watershed water quality standards mandated by PL 95-200. The intent of the standards is to provide baseline water quality values, defined by data collected during a five-year period, against which to compare subsequent measurements.

When the watershed standards were developed, they contained not only values of

water quality constituents that defined compliance or non-compliance, but also administrative requirements for the frequency of compliance checks and specific procedures to be followed in the event of non-compliance. These requirements, as well as the actual development of the standards, forced the functions of the data management system to change from that of simple data collection and archiving to those of analysis, interpretation, and reporting. As these standards have been applied, areas where improvements in the monitoring system could be made have become apparent.

The adoption of formal procedures for analysis and reporting of water quality information has had a number of effects on how data and information are treated. It has caused an information feedback loop to close, resulting in evaluation and subsequent revision of the monitoring. It has resulted in a closer scrutiny of the historic data base, leading to evaluations of its shortcomings and strengths. On the negative side, formal protocols for data analysis tend to foster a rigid, one-track approach to examination of the information. As a result, there is on hand a large supply of data that have been analyzed only one-dimensionally.

It is becoming clear that the greatest need at present is to take a new look at the mass of data collected in order to shed some light on the basic processes that are occurring within the system, and to indicate where to look next. In another example from the watershed monitoring program, a recent analysis of water quality and air quality data suggested that more than half of the dissolved solids load in the water originates from atmospheric inputs. This has important implications in assessing the relative impacts of land use and airshed use on the quality of the water, and leads to questions such as: How representative are the atmospheric input data (collected only at one site)? What are the potential nearby sources of atmoshperic pollution, and what specific constituents might be of concern? These questions, in turn, suggest changes that should be made in the monitoring program and new analyses that should be done.

The problem of formulating process-oriented questions, particularly about meso-scale processes within the system, is that such questions tend not to get asked in the day-to-day operations of such a system. One way to deal with this is to maintain a full-time staff position for the sole purpose of formulating and investigating such questions. Another is to establish a relationship with the academic community where the utility provides some funding and access to data in exchange for research opportunities for graduate students.

SUMMARY

The experience of the Portland Water Bureau has been that the development of a water quality information system is an iterative, cyclical process. The process starts with the need to understand something about the quality of water in the system: to answer the basic question, "What do we have here?" The first step in answering this basic question is to collect samples, or otherwise gather data, and look at what has been gathered. The data will provide some information that suggests more specific questions, shows something that wasn't even looked for, or perhaps suggests that the looking was done in the wrong place, in the wrong way, or at the wrong time. From this point, more data are gathered to investigate the new questions , and the cycle repeats. Examples of this process can be found in a number of facets of Portland's water quality information system.

In the area of data management, the system's starting point was to gather some data for a specific purpose and load it into a computer. Once the data were available on the computer, they were found to be useful. When this utility was perceived, new data continued to be added as they were generated. As new data were added, more efficient ways of getting the data into the computer were conceived, and a greater awareness of the computer's capabilities developed. As these capabilities became apparent, procedures were modified that made the data collection process, with the computer's assitance, more efficient.

As the ability to look at the data for its information content was improved, it became apparent that there were gaps in the monitoring coverage of storm-driven processes in tl watershed. Some sampling was initiated address this problem, and the data generate were examined. The information from th first round of storm monitoring indicated th; the sampling protocols were deficient. Th process is now at the point of investigatir and implementing new sampling technologie -remote sensing and automatic samp collection--to fill in the storm monitorir gaps. As these technologies are implemente they will generate data which will most like dictate further adjustments in the samplin practices.

In a slightly different example, th institution of a formalized analysis an reporting procedure (rather than th institution of a new data collection progran has engendered similar cycles of change. Th process has led to closer scrutiny of both th monitoring program and the historic dat base. Evaluation of the analysis and reportin process, after it had been in use some tim (essentially, after data had been gathered o it), has identified some shortcomings in th process and suggests modifications. Thus, th process has led to a search for new ways c extracting information from the informatio system; seeking new ways of finding the righ questions to ask.

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Systematic Approaches to Monitoring Systems Design

WATER QUALITY MONITORING -- A SYSTEMS APPROACH TO DESIGN

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What is the quality of the water? Can this question, often asked by the public and their elected representatives, be answered by today's water quality monitoring efforts?

The issues raised by the above two questions have been discussed in a number of public forums. The Committee on Science and Technology (1983) held hearings on national environmental monitoring efforts because of their "concern about the condition of the Nation's environmental monitoring programs, programs which are essential both for enforcing existing environmental statutes and for detecting future environmental problems..." Other forums for discussing concerns for monitoring have been the Council on Environmental Quality (1980), the General Accounting Office (1981 and 1986), National Academy of Sciences (1977) and the National Research Council (1987).

In general all the above discussions of monitoring have noted problems with existing approaches. Quite often a specific bias will come through the discussions, but the bottom line is that the design and operation of monitoring systems in the U.S. needs to be based on a more scientific, information oriented, foundation. Water quality management, as with all aspects of environmental management, is becoming increasingly complex as more stringent goals are being requested by the public and their elected representatives. Setting appropriate goals and devising procedures to ensure their achievement (as well as measure such achievement in the environment) are causing a new definition of water quality management that has an insatiable need for information on the behavior of water quality over time and space.

The inability to provide the needed infc mation is documented in many of the abov cited reports. These criticisms have led considerable research on the design of wat quality monitoring systems over the past fi to ten years. In addition, the over: approach to the design of water quali monitoring systems has also been examined

The purpose of this paper is to descril past monitoring system design and operatic practices and then propose a system's fram work to approach such design and operatic that will overcome some of the past dei ciencies. Such a systematic approach is on now becoming feasible as the science and st tistics that are needed to underpin such : information system are now being studied ar formulated in a form that supports such framework.

DEFINITION OF THE WATER QUALITY MONITORING SYSTEM

Water quality monitoring is an effort obtain an understanding of the chemic: physical, and biological characteristics of wat: via statistical sampling. This understandir needs to be cast in the context of tl information needs of the chosen water quali management strategy.

To achieve an understanding of chemic: physical, and biological characteristics (water, samples are collected; analyzed; da from the sample analysis are stored; the da are retrieved and analyzed statistically; repor are written describing the behavior of wat: quality variables; and the reports must the be read and understood. Such a view of

the monitoring system is shown graphically in Figure 1.

CURRENT APPROACH TO DESIGN

Water quality monitoring has historically been viewed as needed to solve a specific problem (ie, a water quality problem must be quantitatively defined so a solution can be formulated). The long term approach of tracking and understanding the behavior of water quality did not fit the concept of "water pollution control" - control pollution on more of a case by case basis. The concept of water quality management is really rather new.

Even as the concept of management of water quality has developed, much of the thinking toward design of water quality monitoring was to simply meet the legal requirement. It is taking time for the true meaning of water quality management to develop and, especially, for its information needs to be defined in a quantitative manner. Millard (1987), and the comments to his paper, present an excellent description of the socio-political setting within which efforts to better quantify environmental monitoring are taking place.

Under the thought that monitoring was required to solve a problem or meet a legal requirement, the focus for design generally revolved around the need to design a monitoring network. In other words, where will we sample, what will we measure, and how fre- quently will we take samples. Once these three factors of network design were decided (but rarely documented), samples were collected, samples were analyzed, and data was placed in files.

The data were not analyzed on a regular basis, but rather when necessary.

CHARACTERISTICS OF ILL-FATED NETWORK DESIGNS

Perhaps the major characteristic of a monitoring system, that is doomed to failure, is the lack of an "information" reason for existing! The water quality information goal(s) are not defined in any quantitative, documented fashion. No one knows exactly

what is to be done with the data, much less how it is to be done.

This fact does not prevent attempts to get "information" from the monitoring system by taking the data to a statistician, placing it at his or her feet, and asking, "What does the data say?" This is almost an impossible situation - there are missing values, non-detects, outliers, multiple samples per sampling interval (part of a QA/QC effort), multiple sampling frequencies over the record, and no documentation as to why or how the data were obtained. In other words, the statistical sampling effort was not designed properly in the first place and now we are hoping statistics can come to the rescue! Ross (1987) discusses the fact that statisticans are not completely blameless in this situation. Their expertise needs to be taken to the water quality management field and employed in a less than perfect situation.

What data analysis techniques are to be used to analyze the water quality data? What type of information is desired? How do you want the information reported? How do you want to deal with the above data record limitations? These are all questions that need to be answered before any meaningful data analysis can proceed. These are also the same questions that should have been answered as part of the initial monitoring system design effort - before the first sample was collected.

Thus, when critiquing an existing monitoring system that is a part of an ongoing water quality management effort, one should look for:

1. Defined and documented water quality information goals

2. Network design that is documented

3. Defined and documented data analysis procedures (protocol)

4. Defined and documented reporting mechanisms

Without the above issues being defined, it is very difficult to obtain information from a

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Figure 1. The Water Quality Information System

monitoring effort. There is little connection between data collection and data analysis that is apparent to the personnel operating the monitoring effort. Quality control/quality assurance focuses on one sample at a time and not the information to be produced. Likewise, data storage deals with storing numbers, not on preparing a data record for future data analysis. Without documented reasons for the form and operation of a monitoring program, there is little resistance to changing the monitoring system at the personal whim of a future manager. The resulting broken and incomplete records, over time, generate little or no useful information. None was designed to be obtained and none is being obtained!

The design and operation of a poorly conceived monitoring system focuses on the collection of data and not the creation of information. In a well designed and operated monitoring system, the information purpose or goal guides the definition and execution of all activities in the information system.

FRAMEWORK FOR DESIGN OF A WATER QUALITY INFORMATION SYSTEM

How does one go about designing a water quality monitoring system that focuses on producing information rather than data? It should be pointed out that this is an area of intense research by a number of people, and the ideas presented in this paper are but just one suggested approach. It is an approach that has been successfully utilized in a number of monitoring system designs and evaluations.

Perhaps the most critical factor in the design of a water quality information system is viewing monitoring as a system. The system presented in Figure 1 is the overall perspective that underpins the framework being suggested here. All facets of the system in Figure 1 must be thoroughly defined.

Within the monitoring (information) system, an equally important factor in design is quantification of the information goals. What is the management goal that requires monitoring? What is an appropriate, corres-

ponding information goal for the monitoring system? How is "water quality" being defined in this monitoring (information) effort? What statistical "hypothesis" captures the essence of the information goal? What statistical "test" is most appropriate to test the hypothesis and yield the desired information? What sampling plan best provides the data required by the chosen statistical test? What wording is most appropriate for the final "conclusions" drawn from the data analysis?

Answering the above questions, step-by-step, leads one to much more quantification of information goals and a stronger scientific basis for design of the overall water quality information system. The use of statistics provides a common "language" for quantification (among the many professions involved in water quality management today) and permits development of statements about the uncertainty associated with the inferences being made about a water quality "population" using a few samples. To further illustrate this quantification of information "expectations", Figure 2 contains two very brief summaries of the steps that could be involved.

The statistics chosen above, based on the information desired, may not match the statistical and available data set limitations (such limitations are often an indication of the type of problems to be expected in future data analysis). Thus, after completing the above information "expectation" assessment, it is necessary to evaluate the statistical behavior of the water quality variables being measured (such as serial correlation and seasonality) and the data set limitations to be encountered (such as missing data, non-detects, and multiple observations in one sampling period). Such an evaluation may indicate that the statistical methods chosen to analyze the data are invalidated by the data characteristics. In this case, it will be necessary to iterate back to the information expectation phase of the monitoring system design and "adjust" the information expectations in light of the ability of the monitoring system to supply data.

Once the information to be obtained and supporting statistics are defined, it is possible to begin the network design phase of the monitoring system design process. Here the

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Quantifying Information Expectations

Management Goal: Maintain or improve water quality

Monitoring Goal: Detect trends in water quality

Definition of Water Quality: Dissolved oxygen, nitrates, and total
dissolved solids

Statistical Methodology: Linear regression fit of data versus time

Statistical Hypothesis: Slope of linear regression line is zero at 95% confidence level

Monitoring System Product: Conclusions regarding slope of regression line

Reporting: Management goal is met when all slopes are zero or indicate
improvement

Quantifying Information Expectations

Management Goal: Contain plume

Monitoring Goal: Detect trends in water quality

Definition of Water Quality: TCE

Statistical Methodology: Gradual trend   Step trend
                              - Kendall's Tau   - Mann-Whitney

Statistical Hypothesis: H_o: No trend
                              H_a: Trend exists

Monitoring System Product: Conclusions regarding presence or absence or a trend over tim

Reporting: Management goal is met when either no trend or trend towal
decreasing concentrations of TCE exist at all wells

Figure 2. Examples of Quantifying Information Expectations

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exact locations for sampling are defined and the frequency of sampling is established at each sampling site. Of course the information objectives will greatly influence sampling location and the frequency of sampling often falls out of the statistical analysis performed to validate the chosen statistics. The exact water quality variables to measure are decided at this point using the definition of water quality developed in the information expectation phase of the system design process and any correlation that may exist between variables.

The exact procedures to be used in the day-to-day operation of the monitoring system need to be documented throughout the entire system. From preparation of sampling routes and specification of sampling protocols through identification of standard laboratory analysis methods to definition of data handling and storage procedures, the operating procedures need to be documented in detail. To leave portions of the monitoring system undefined or poorly defined, is to leave open the opportunity for inconsistent operation of the monitoring system. This permits introduction of variability into the data that comes from the operation of the monitoring system and not from the behavior of the water quality variables.

Data analysis, reporting and information utilization "protocols" also need to be defined as part of the monitoring system design. Specification of this final information generation phase of the monitoring system is where considerable uncertainty in the design process exists. Specification of the information expectations in a quantitative fashion, with corresponding statistics, forms the basis for preparation of a data analysis protocol. Reporting and information utilization "protocols" will be highly dependent upon the exact nature of the management effort and the way it is organized to incorporate information on the behavior of the water quality it is managing. Establishing reporting and information utilization protocols will require a rather close examination of decision making within a management organization.

The above framework for designing water quality information systems can be summarized in a five step process as noted in Figure 3.

COSTS OF PROPER SYSTEM DESIGN

To execute the above water quality information system design framework will require considerably more expense up front in a monitoring effort than has historically been provided. The best way to view the costs of design is in the context an engineering project. We would never consider constructing and utilizing a building or bridge without initial engineering design. And yet we will, over a period of say 10 to 20 years, operate a water quality monitoring system without proper initial design. If the cost of operating the monitoring system is $250,000 per year, then the total cost of the information obtained amounts to $5 million over a 20 year design life (not accounting for interest or inflation). If 10 percent of a project is to be used for initial design (which is common in many engineering projects), then $500,000 for initial design of the water quality information system is not out of line. Considering the amount of work involved in executing the framework described above, then one can also see that the $500,000 is realistic relative to the tasks involved.

The result of expending the above design costs should be a water quality information system design document. Such a document is the result of expending the design money and serves to communicate to everyone involved in the information system exactly what is to be produced, in addition to defining the exact procedures utilized to produce the information product. Thus, it is easier to justify the initial design costs when a thorough design document is to be the result of the expenditure.

INFORMATION PROTOCOLS

Water quality monitoring today employs sampling protocols, QA/QC protocols, standard laboratory methods, data storage and retrieval protocols. It is time to complete standardization of the complete monitoring system by developing "information" protocols. Ward et al (1988) suggest a data analysis

STEP 1   <u>Define Information Expectations</u>

- Determine management and corresponding monitoring goals
- Define water quality for monitoring system design purposes
- Identify statistical methodology to be used by monitoring system
- State statistical conclusions to be drawn from data and discuss how these conclus relate to management goals
- Describe means of reporting conclusions

STEP 2   <u>Confirm Statistical Design Criteria</u>

- Statistically characterize water quality "population" to be sampled
    - --plot concentration and flow versus time
    - --normality testing variance homogeneity testing
    - --independence testing
- State that assumptions of chosen statistical methodology are met

STEP 3   <u>Design Monitoring Network</u>

- Where to sample (from management/monitoring goals)
- What to measure (from water quality definition and management/monitoring go;
- How frequently to sample (from needs of selected statistical methodologies)

STEP 4   <u>Develop Operating Plans and Procedures</u>

- Sampling routes, equipment, and employee training
- Field sampling and analysis procedures
- Sample preservation and transportation
- Laboratory analysis and quality control procedures
- Data verification protocols
- Data storage and retrieval hardware and software
- Data analysis software for chosen statistical methodology

STEP 5   <u>Develop Information Reporting Procedures</u>

- Type, format and frequency of reporting
- Distribution of reports
- Automation of reporting
- Evaluation of information relative to expectations defined in Step 1

Figure 3. Water Quality Information System Design Framework

protocol for ground water quality monitoring systems employed for management of water quality at an industrial site. The Water Resources Council (1977) has suggested standard methods for determining flood flow frequency. Harcum (1989) has examined many of the issues associated with developing standard water quality data analysis protocols and concludes that there is considerable additional work needed before such documents can be prepared with confidence. That does not mean that a data analysis protocol can not be prepared, using best available information, and incorporated into the design of a total monitoring system. It does mean that as data become available from the monitoring system, provision for periodic evaluation of data analysis methods needs to be incorporated into the initial design.

Reporting protocols should deal with such issues as frequency of reporting, content of reports, format for presenting information, distribution of reports, targeted audience, indication of the general form of the conclusions to be presented in each report, means to evaluate the reporting process, and plans for automation for the entire reporting process. This last point deserves considerable attention in the initial design of a total monitoring system. Developing reports from monitoring efforts usually involves considerable staff time. Finding the time to put the data in a form for analysis, deciding which data analysis methods to use, selecting a computer and software system for the analysis, performing the computer operations, putting the results in an acceptable format and deciding who should receive the report, all take considerable staff time.

Because of the large time commitment to prepare a report, reporting is often slighted in favor of collecting more data! The problem here is that the staff, after the monitoring system has been operated for a number of years, is being asked to complete the design of the information system while also trying to continue its operation. The true cost of monitoring system design is extracted from the staff many years after the system began operation. If the reporting protocol was designed at the beginning of the monitoring effort, then reporting should be incorporated into the day-to-day operations and becomes another task to be completed on a regular basis. In addition, the procedures for reporting should be readily available to the staff.

Issuing reports may often be viewed as completion of the water quality information system. However, the view taken here is that until the information is utilized to improve the management operation, the system's true objective is not completed. Thus, the ultimate use of the information needs to be defined for the users of the information! This effort to define utilization of water quality information may show that such information is not needed. Or it may reveal that many management decisions are made for political and economic reasons rather than water quality reasons. In this latter case, we must ask ourselves if the money spent to obtain water quality information is necessary. Developing a water quality information utilization protocol can be a very revealing exercise and one many managers may be unwilling to undertake! However, if monitoring systems are to be justified in the context of helping provide information for better decision making, then such protocols are needed.

The above discussion has touched on some of the reasons that "information" protocols are needed. In summary, the reasons for "information" protocols are as follows:

1. They complete documentation of the system design through ultimate use of the information

2. They permit "auditing" of the data analysis methods, reporting mechanisms, and the ultimate utilization of the information

3. They introduce consistency of data analysis, reporting, and information utilization among sites and personnel over time

4. They can incorporate state-of-the-art knowledge into the monitoring system design and operation

INFORMATION TO BE PRODUCED

What information can we expect from a water quality monitoring system? First, it is important to remember that it is difficult for one monitoring system to answer the "what" and "why" questions at the same time. So normally, one would design one system to answer the question, "What is the quality of the water?" Once the quality of the water is defined, the next question, "Why is the water quality what it is?" This paper deals much more with the first question in that it is envisioned such a monitoring system provides a management effort with the tracking required to properly evaluate its use of management resources and overall achievement of water goals. When the answers to the "what" question reveals a problem, then the "why" monitoring, often in a more flexible operation (ie special studies) comes into play. The two types of monitoring complement each other within a management effort.

In answering the "what" question, a monitoring system can, in a highly generalized manner, be considered to provide information on three characteristics of water quality:

1. Average water quality conditions

2. Changing water quality conditions

3. Extreme water quality conditions

Presentation and interpretation of such water quality information in terms of management goals becomes the goal of the reporting and utilization portions of the monitoring system.

Taking the average, changing and extreme behavior of water quality and interpreting it in the context of management decision making may cause some problems. A water quality report noting degrading water quality conditions in a state may become the center of a political campaign. The reporting of environmental conditions and trends has not reached the acceptability of the reporting of economic conditions and trends. The political heat of a "negative" water quality report may result in the water quality management agency forced to cease monitoring, or at least reporting such information. Information

protocols can help address many of these potential problems.

CONCLUSIONS

Strategies to improve the design of water quality information systems are available; however, there are not many documented applications of such strategies in practical settings. While this paper has outlined one such strategy, it is left to other papers in this symposium to describe applications to practical situations. In listening to the efforts of others to design effective monitoring systems and to provide more science to specific aspects of a monitoring system, it is useful to keep in mind the totality of effort needed to design and operate a successful water quality information system. That totality has been summarized in this paper with emphasis on the "information" portion of the system.

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WATER QUALITY BRANCH MONITORING ACTIVITIES - A DYNAMIC APPROACH TO EVOLVING ISSUES -

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The Water Quality Branch (WQB), Inland Waters Directorate, Department of the Environment (DOE), provides scientifically sound information related to Canada's freshwater resources for government, private agencies and the general public. The WQB is the sole federal agency responsible for the development and operation of water quality monitoring networks to assess the quality of the ambient aquatic environment. This includes the identification of problem areas, promoting research related to inland waters, and the planning and implementation of water programs and policies. The WQB is operational in nature, research services are provided by the National Water Research Institute and the National Hydrology Research Institute .

Although water management responsibilities are shared with the provinces, the federal government provides leadership, particularly when addressing national water quality concerns. The Department does, however, participate with the provinces in water management programs involving transboundary waters and other waters of federal interest.

Federal Policy Statement No. 9 (1978), committed the Department to monitor the quality of water at international and interprovincial sites, Indian reserves, national parks and other areas where there is significant national interest. As a result, data from non-boundary waters within the provinces and territories was not collected as it was considered to be outside the Department's mandate. The problems associated with this approach, particularly the inherent lack of consistency and areal coverage in data collection, were identified in the 1980 Auditor

General's Report. This situation was resolved in 1982 by a federal cabinet decision which authorized DOE to negotiate water quality monitoring agreements with the provinces, enabling the department to obtain data on ambient waters within the provinces .on a cooperative basis. The Federal Water Quality Monitoring Agreements which evolved from this decision effectively linked federal and provincial monitoring activities, thereby ensuring long term commitments to provide compatible data bases, accurate information and comprehensive water quality assessments on a national and regional basis. The agreements also serve as a mechanism to promote federal-provincial cooperation.

Within this framework, it is necessary that monitoring activities satisfy the requirements of the Federal Policy Statement. A broad range of water quality related issues have been identified in Canada that require information on a national scale. Of particular note are those issues identified by the Canadian Council of Resource and Environment Ministers, CCREM (1985), listed in Table 1 in no particular order of priority.

Subsequent to this, the Department identified a series of water related priorities which are presented in Table 2. The priorities are not congruent and reflect the scope and diversity of water quality concerns in Canada.

In order to be able to address the varied water quality issues that Canada is facing, it is necessary to develop comprehensive water quality monitoring networks capable o providing requisite data that are scientifically defensible. Due to the multiplicity of data

TABLE 1

Canadian Water Quality Issues as Identified by the Task Force of the Canadian Council of Resource and Environment Ministers (1985)

1. Pollution of waters used for recreational purposes.
2. Contamination of water supplies for drinking water purposes.
3. Impact of land use practices on water quality.
4. Impact of toxics and other contaminants on aquatic environments.
5. Impact of water-related development projects on the aquatic ecosystem.
6. Impact of LRTAP (long range transport of airborne pollutants) on water quality.
7. Chemical contamination of fish.
8. Public perceptions of water quality.
9. Conflicts over water quality uses.

TABLE 2

Department of the Environment Priorities (1988)

1. Federal Water Policy
2. Canadian Environmental Protection Act (CEPA)
3. Great Lakes Clean-Up
4. Acid Rain Impacts
5. Flood Damage Reduction
6. Water Quality Monitoring Agreements
7. Ground Water Contamination
8. Toxic Chemicals Research
9. Mackenzie and Yukon River Basin General Agreements
10. Environment Economy
11. State of the Environment Reporting

needs, the assessment strategy of the WQB must be flexible.

No single network can be designed to address all issues nor supply the same quality of information for all issues. At first glance, it may appear that this would result in a number of diverse and poorly related networks; however, there are unifying elements inherent in the design concepts of all networks. Other components common to each network include quality assurance protocols, compatible analytical and field sampling methodologies, common database management and centralized data archiving.

Historically, water quality assessments were based on fixed station networks with water samples collected at set frequencies (weekly, monthly or quarterly). Although useful as a means of developing an inventory of water chemistry data, such networks have proven to be inadequate to determine the state of the aquatic environment or to establish water quality objectives. This "do everything-everywhere" approach (Great Lakes Science

Advisory Board, 1978) is detrimental and lacks the flexibility required to adequately address all water quality issues.

Haffner, (1986) discussed the WQB's acceptance of river basins of federal interest as being the basic sampling units across Canada. Using river basins in this manner permits the use of fixed network and survey approaches as environmental quality assessment tools. Each method has distinct advantages and disadvantages. Often considered as alternatives, they are best considered as being complimentary mechanisms to obtain environmental data. The WQB uses the river basin approach to provide comprehensive assessments and to secure appropriate information for river basin planning and management activities. The choice of basins to be surveyed and the priority for the implementation of each study is dictated by a number of factors which include the following:

(1) the probability that changes in water quality are occurring or will occur;

(2) the need to develop background information concerning the status of ecosystem quality;

(3) the identification of emerging issues (research community, etc.); and

(4) the importance of the basin with respect to real or potential water quality concerns.

To be consistent with the Federal Policy Statement, the design of each network must be such that appropriate data are obtained to:

(1) establish baseline information;

(2) identify water quality trends on a national and regional scale;

(3) determine whether water quality objectives are being met;

(4) assess the effectiveness of regulatory measures in achieving the desired level of water quality; and

(5) provide a basis for revising control requirements where nc

While many of these objectives ; related, it is obvious that there is a more than one assessment approac example, the WQB addresses objecti\ 3 by using fixed station networks, objectives 2,4 and 5 are addressed survey component in the monitorin To fulfill its mandate the WQB h; mined that the basin sampling strat combine both fixed station and approaches. Specifically, these netw referred to as index station netwc recurrent river basin networks. approaches differ in that the former an assessment of long-term, averaç quality conditions and seasonality, wht latter provides information on the mental significance of water quality cc (Haffner 1986). Stations addressin national or interprovincial water quali will usually be index stations dependin type of information required. Other selected to monitor water quality is federal lands or interprovincially may to either category.

Index Station Network

The index station network is a net fixed stations geographically distribute Canada at strategic locations withi basins of federal interest or alon dictional boundaries. They are sam regular intervals (quarterly to month the long term to describe baseline cor indications of change or long-term The stations are called index stations their location within each river basin c body should be such that they pro indication of change in water quality the basin which may warrant more com sive water quality monitoring to detern cause and effect of the change. Index also provide an indication of improven water quality over the long term as a r implemented remedial actions. Station are part of this network also form an part of the recurrent river basin programs carried out within each regic basins identified for surveys will

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contain an index station to maintain continuity between the recurring survey periods.

Recurrent River Basin Network

A comprehensive network of fixed (permanent) stations throughout Canada would be very expensive, and similar approaches have been criticized as being relatively inefficient to meet the dynamic nature of water quality issues (GAO, 1981). Although the need for a fixed station (index) network exists, it is important that it be complemented by periodic recurrent surveys. In general, basin monitoring is directed toward understanding the behaviour of the basin system (i.e., cause/effect relationships), determining the sources and impacts of pollution and identifying existing or emerging water quality concerns. The strategy for the recurrent river basin survey provides the capability of assessing water quality problems in a dynamic, comprehensive manner. Most importantly, the development of water objectives and the assessment of the aquatic environment with respect to these objectives requires a survey approach to determine frequency of violations of water quality objectives, areal extent of the problems and the identification of possible remedial efforts.

Federal and provincial agencies have concentrated their monitoring efforts in the past on a more or less standardized list of ambient physical and chemical parameters. This approach has been well established in Canada. However, a need for change has been recognized for some time. Harvey, (1976) indicated that "A disproportionately large effort is devoted to monitoring water chemistry and fish physiology/toxicology and this could be reduced. The effort expended on ecosystem approaches is small and should be increased". The ecosystem approach has gained wide acceptance in Canada and to this end the WQB has augmented its parameter lists with the addition of biological parameters. The use of biota and sediments to measure trends in toxic substances has become well established.

The National Reference Network (NRN)

Due to increasing public anxiety concerning the quality of Canada's freshwater supplies, the WQB is presently developing a strategy for the design of a network which will address issues on a national scale. The network, issue driven by nature, will be referred to as the National Reference Network (NRN), and will provide scientific information and advice on selected water quality issues. For the purpose of this network a national issue has been defined as either:

"a water quality concern that is of sufficient import to potentially threaten, or impact surface water resources across Canada or, a regional problem that is of sufficient import to capture national attention".

Monitoring is defined as "the process of repetitive observing of one or more elements or indicators of the environment according to prearranged schedules in space and time, using comparable methodologies for environmental sensing and data collection" (Pierce et al. 1982).

In accordance with Ward et al., (1986), the first step in creating the NRN was the establishment of management goals, which will determine the resulting monitoring objectives for each issue and, ultimately, the network design. For example, if the management goal is to "protect (or maintain) and improve (or enhance) water quality in Canada", then the monitoring objective will be to ascertain changes or lack thereof in water quality over time (i.e., trends). Sites will be selected to be "representative " of Canada's water resources and in accordance with an "area at risk" predictive model. Sampling frequency will be related to trend detection (i.e., fixed interval or systematic sampling) and parameters selected for monitoring will be based on the operational definition of water quality. If on the other hand, the management goal of the program is to "promote the conservation and best use(s) of natural waters", then the

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monitoring objective will be to ascertain compliance or adherence to water quality objectives or guidelines for the detailed water use. In this case, sampling sites will be concentrated where water use conflicts are anticipated, sampling frequency will be related to the detection of non-compliance (i.e., non-systematic sampling, which is unsuitable for trend detection). Parameters will be related to the water quality requirements of the defined uses. These goals are not mutually exclusive, but it is important that they are clearly understood at the outset so as to ensure that the network design is in accordance with management expectations for each particular issue.

The process of translating the various management goals into viable water quality monitoring programs will closely follow the steps outlined by Ward et al. (1986):

Step 1. Translate the management goals into quantifiable monitoring goals (as statistical hypotheses).

Step 2. Establish the statistical criteria to each of the hypotheses.

Step 3. Design the monitoring network i.e., the where, what and when of monitoring.

Step 4. Develop the operating plans and procedures i.e., sampling protocols, QA/QC, data analysis software, etc.

Step 5. Develop the information reporting procedures e.g. type of report, define audience(s), frequency of reporting, etc.

Ideally the results produced will enable the WQB to relate the occurrence and concentrations of the various chemicals studied to the surrounding environment and to increase the probability of extrapolating findings to other areas which are not monitored.

It has been noted that our ability to assess water quality changes in aquatic ecosystems has been limited by the absence of long-term data sets which have prevented the definition of the normal range of critical measurable

variables (Schindler 1987). Conseque is essential that the NRN be suff inexpensive so as to withstand bu constraints and hence be continuou extended periods of time. To meet thi it is envisioned that the proposed NR be entrenched where possible into e federal-provincial water quality moni agreements.

The problem of maintainin, comparatively simple monitoring netwc the face of increasingly challe environmental issues requires that the be integrated with regional water q assessment programs. The NRN will chiefly as a means of problem identific and priorization from a national perspe Where potential water problems are indic regional programs, such as recurrent basin studies, will be undertaken that assess the magnitude and scale of the pro utilizing sampling protocols consistent those of the NRN.

Issues To Be Addressed By The Nati Reference Network

1. Definition of pristine or bas conditions in all ecoregions Canada.

2. Impact of agricultural pesticides adjacent aquatic ecosystems.

3. Impact of urban and indust contaminants on adjacent aqu ecosystems.

4. Long-range transport of airbo pollutants (acid rain, organics).

5. Impact of eutrophication on adjac aquatic ecosystems.

Each issue will be treated independent leading to a number of issue-speci networks, each designed to meet the go established for the issue. In this way, statio will only be used for specific purposes, th eliminating the collection of redundant superfluous data. To demonstrate t approach being used, details for t

development of the network for issue 2 are presented.

STATEMENT OF THE PROBLEM

Agricultural practices in Canada rely heavily on chemical pesticides to control pests and crop diseases. The use of herbicides, insecticides and fungicides has contributed to large increases in agricultural yield and productivity in Canada over the last 40 years. This success, however, has not been attained without a price in terms of adverse environmental impacts on non-target organisms. Generally, less than 1% of a pesticide applied to crops impinges on target organisms. This percentage is even lower due to improper application, a not infrequent occurence (Pimental and Levitan, 1986).

Pesticides can reach water supplies through a number of avenues including, but not limited to, overspray, aerial drift, surface runoff, leaching and spills. Unfortunately, the potential hazards associated with the presence of these pesticides in surface waters is difficult to assess, since information regarding the presence and fate of these chemicals is not well documented. Basic water quality information regarding the presence and concentration of this group of compounds in high risk watersheds is needed to:

(1) determine whether it is likely that environmental quality in these waters is adversely affected by the use of these pesticides; and

(2) determine whether any existing water quality objectives are being exceeded.

The management goal identified for this issue was "to encourage the maintenance and enhancement of surface water quality consistent with the use(s) of these waters". This translated into the following monitoring goals:

(1) Are levels of agricultural pesticides detectable in waters or sediments adjacent to areas of high agricultural activity during periods of high probable impact (i.e. presence/absence after application; and

(2) Where detected, are the levels of agricultural pesticides present in concentrations that are deemed harmful to the aquatic ecosystem?

At this stage in the development of the network only problem identification and characterization are being considered, little time has been devoted to the next step which will focus on the requirements of a program designed to accurately monitor trends or to define the extent of the problem.

The microcomputer based geographical information system (G.I.S.) SPANS was used to develop predictive models for each of the Canadian provinces. Specificially, the models were used to identify areas of high risk, i.e. areas where pesticide use may have potential impacts on water quality. SPANS offers a unique opportunity to incorporate various pieces of information into visual (map) forms. In the development of the predictive model, various information items were obtained from Statistics Canada and the Environmental Information Systems Division, Environment Canada. Map and attribute information requirements were incorporated as follows:

Maps: Provincial Base maps
     Census Consolidated Sub-Division maps
     Watershed Sub-Divisions
     Land Capability for Agriculture

Attributes:
     Land Capability - primary class;
     Census of Agriculture - Pesticide Use (Land area sprayed or dusted)
     Census of Agriculture - Farm Area (Improved, unimproved, total)
     Land area per CCSD - from SPANS area analysis.

With this information, a series of steps were taken which resulted in the production of a pesticide impact area map (an indexing overlay of the land capability, agricultural activity and pesticide use maps) to give a composite picture of the pesticide usage expected within agricultural areas. Following this, an overlay of the impact area map onto the watershed map was made. Finally, a report from the unique conditions file was

watersheds having significant impact ratings, as well as what percentage of the total watershed these areas represent.

With river basin areas now identified, the siting of sampling locations was undertaken. Specifically, questions concerning which pesticides are used, when they are applied and where their products are expected to be detected (i.e. ground water, discharge areas, etc.) were addressed. Sampling frequencies, parameter lists and other field sampling considerations were then incorporated into the design.

This process will be repeated for each of the issues identified. It is hoped that this approach will ensure a linkage between the WQB's monitoring programs and, consequently, contribute data of an appropriate nature to meet specific information requirements.

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MONITORING TO IMPROVE DECISION-MAKING IN EPA AND STATE SURFACE WATER QUALITY PROGRAMS

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WHY MONITOR?

The ultimate objective of the Federal Clean Water Act is to improve the environment - "to restore and maintain the chemical, physical, and biological integrity of the Nation's waters." In the early years of the Clean Water Act, when sources of pollution were easily identified, instream impacts obvious, and the solutions proven, we could be reasonably confident that efforts to regulate environmental pollution would result in progress toward the Act's environmental objective. In these cases where there was little doubt about the problems or the solutions, low priority was given to measuring the extent to which regulatory efforts actually improved the environment.

Today, however, we face water quality problems whose sources are diffuse, impacts subtle, and solutions unproven. This uncertainty makes it less obvious which pollution sources need to be further controlled, what level of control is needed, or how effective a control effort will be as measured by actual improvements in environmental quality. To overcome these uncertainties and ensure that we are cost-effectively improving the environment, we need information about the environment: to warn of emerging problems; to accurately locate problem areas where the greatest environmental good can be achieved; to set discharge limits at levels sufficient to protect instream uses (but to avoid unnecessarily stringent limits); and to verify that the assumptions used in the regulatory process hold true to produce measurable improvements instream. Each of these decisions or program actions can be improved with the consideration and/or use of monitoring information (i.e., information about the environment).

The type of monitoring information needed varies according to its intended use. The types of information used or considered in water quality programs include measurements of: the physical/chemical quality of water, sediment, and tissue; effluent and ambient toxicity; the health or integrity of resident biological communities, and the condition of the physical habitat.

USES OF MONITORING INFORMATION

The uses of monitoring information in water quality problems can be categorized into four broad program areas: (i) developing water quality standards; (ii) planning and problem identification; (iii) making control decisions; and (iv) evaluating program effectiveness.

Developing Water Quality Standards

The first program area in which monitoring information can improve decision-making is in the development of water quality standards. Monitoring information can be used to help translate the Clean Water Act's objective of chemical, physical, and biological integrity into workable and locally meaningful water quality goals or standards. Developing and refining standards can involve:

- refining aquatic life use classifications in State water quality standards;

- identifying and characterizing "least impaired" reference conditions to develop site-specific, regional, or statewide criteria (including biological criteria); and

- conducting "use attainability analyses" to assign use classifications to individual waterbodies or waterbody segments (including the identification of high quality waters deserving special protection).

Planning and Problem Identification

Monitoring information can also help in planning and problem identification. It can help discover previously unrecognized water quality problems; identify worsening trends that warn of emerging problems; set priorities within and between programs; and develop management plans. Monitoring information can be collected at different geographic scales to:

- screen large geographic areas for suspected or emerging water quality problems and identify probable sources and causes of the problems (e.g., in entire watersheds or estuaries);

- and to confirm suspected water quality problems and diagnose the specific causes and sources of impairment.

Making Control Decisions

Monitoring information can also improve individual regulatory (or other control) decisions. It can increase cost savings to the regulated community through better wasteload allocations and modeling, and document the need for regulatory actions to avoid legal challenges. Monitoring information can be used to help:

- determine appropriate NPDES permit limits in water quality limited segments;

- conduct Clean Water Act §401/404 certifications and reviews; and

- support the development of Super-fund/RCRA action plans.

Evaluating Program Effectiveness

Lastly, monitoring information can be used to evaluate the effectiveness of water quality

programs in restoring degraded areas maintaining clean areas, and demonstrat environmental benefits of abatement acti an era of constant or dwindling reso Monitoring information can be used to

- evaluate compliance with conditions or decisions to impl Best Management Practices to cc that management actions are ins and maintained (i.e., *implementa monitoring*);

- evaluate the extent to which c efforts improve the environment result in the restoration maintenance of water quality star (i.e., *effectiveness monitor.*

- evaluate the extent to which allocation of program resources funding, staffing) to different cate of pollution sources, different geog areas, or different ecological s makes sense in light of environmental impact addressed;

- assess regional or statewide trei determine whether water quality (health of living resources) is impr merely keeping pace with growt development, or degrading.

Who monitors? Who uses monitoring information?

The U.S. Environmental Protection / (EPA) and State water quality agencies primary responsibility for implementii Federal Clean Water Act. It is the however (and interstate agencies anc territories), who make most of the "pr(matic" decisions (e.g., developing water standards, determining discharge limit: could benefit from use and/or considera monitoring information.

Accordingly, the biggest collectoi users of monitoring information are water quality agencies. Virtually all conduct special studies or surveys maintain some sort of fixed station n which they regularly sample, althougt

monitoring programs vary tremendously in size, capabilities, and design. EPA often assists States in monitoring, as do the National Oceanic and Atmospheric Administration, the U.S. Geological Survey, the U.S. Fish and Wildlife Service, the U.S. Forest Service, the Soil Conservation Service, State fish and wildlife agencies, volunteers, permitted dischargers, and others. EPA and States in turn analyze and report information not only for internal use but to inform the US Congress, State legislatures and regulatory control boards, local agencies, the public, and the regulated community about water quality goals, problems, and solutions.

What has EPA's role been in ensuring the adequacy of State monitoring programs?

States vary widely in the extent to which they collect monitoring information and use monitoring information in management decisions. Some variability is to be expected since State information needs vary depending on the extent and nature of a State's water resources, pollution sources, past abatement efforts, past monitoring, funding, staffing, available technical skills, and other factors. But there seems to be a consensus that some State monitoring programs are inadequate, and that the deficiencies stem in part from a lack of national direction that EPA only recently has begun to remedy.

The Clean Water Act itself offers little direction on monitoring. It requires numerous program actions and reporting activities that can and often are based on monitoring information, but provides little explanation of what monitoring information is needed to support these activities. The Act dictates only that States establish and operate "appropriate devices, methods, systems, and procedures necessary to monitor, and to compile and analyze data on ... the quality of navigable waters."

It is through regulations, policies, and guidance that EPA can define elements of what it considers to be an adequate State monitoring program. In practice, EPA has relied on guidance and statements of policy rather than regulations. EPA's one attempt

to develop detailed surface water monitoring regulations failed because the regulations attempted to define too many technical details about how States were to choose station locations, parametric coverage, and sampling frequencies.

Instead, EPA has expressed its view of what constitutes an adequate State monitoring program through statements of policy and guidance. EPA issued a monitoring policy in 1984 which identified EPA's highest priority monitoring objective to be the establishment of water quality-based permit requirements and the determination of needed nonpoint source abatement actions. EPA has issued national monitoring program guidance in 1975, 1977, and 1985 (supplemented with §305(b) guidelines every two years and EPA's annual Operating Guidance) on what constitutes an adequate State monitoring program. EPA Regional Offices also play a major role in interpreting and supplementing national guidance. Past guidance has included various recommendations such as for States to conduct intensive surveys to develop discharge limits for permitted point source dischargers; or to assess all waters at least once every five years. The recommendations made in previous guidance are currently under review.

One interesting effort established by the 1975 program guidance was the joint development between EPA and the States of a 1,000+ station ambient water quality "core network." Its purpose was to allow EPA and others to prepare independent national analyses of water quality. The effort failed for reasons that remain unclear, but appear to have included poor design (e.g., station locations were selected through negotiation rather than a predetermined statistically representative design). In addition to developing policy and "programmatic" guidance, EPA also assists States with technical guidance, data system capabilities, training, and other assistance.

How can EPA/States improve the utility of monitoring information?

EPA is working with States to provide new and updated statements of policy, revised programmatic guidance, various technical

guidance, new data system capabilities, training, and other assistance to improve State monitoring programs.

The monitoring program guidance will encourage the use of monitoring information in more than ten distinct water quality program areas and offer States general program design recommendations including:

- conduct watershed-level assessments that facilitate the identification of sources of pollution that would benefit most from controls, better account for interactions between dischargers, and increase the chances of detecting and documenting environmental improvement;

- conduct integrated assessments (using chemical analyses, toxicology, habitat evaluations, and biological surveys) capable of detecting a wide range of water quality problems;

- maximize monitoring resources by taking advantage of interagency coordination, ambient monitoring by dischargers, volunteer monitoring; exploring alternative sources of funding; and making use of existing water quality data and predictive modeling techniques;

- involve citizens in identifying problems and working toward solutions to increase their sense of responsibility for our publicly-owned natural resources;

- interpret and analyze monitoring data to present it in a readily useable form;

- improve water quality criteria and standards since the interpretation of ambient data generally requires comparison to a reference, or control.

Other efforts underway to improve EPA/State monitoring programs include:

- a policy on the use of ecological assessment methods and biological criteria in EPA/State water quality programs;

- guidance on using volunteers to co monitoring information;

- technical guidance on nonpoint so monitoring and evaluation, biolo assessment methods, and other top

- periodic symposia to exch information and build conse between Federal and State agencie monitoring methods and issues;

- a multi year plan for the Water Q Standards Program which will enco States to supplement traditional column chemical criteria with column toxicity criteria, sediment q criteria, habitat quality criteria, biological criteria;

- new data system capabilities.

CREATING A MARKET FOR DAT

In addition to working to strengthen monitoring programs to ensure that produce the type and quality of inforn needed by decision makers, EPA is working to increase the incentive for EP State managers to base program actio their environmental consequences. E attempting to supplement the way historically judged the performance Regional offices (which oversee State quality programs) by using environ measures, rather than just adminis measures, to set annual program goa track progress toward achievement of goals. Typical administrative measures numbers of permits issued or re enforcement actions taken, or administered. These measures do i progress but they do not guarantee effective improvements in environ quality. Environmental measures measures of biological community st and function or the presence of toxici

EPA's new Administrator, William has in fact declared that each of programs will set long-term enviroi

indicators of environmental accomplishments to evaluate the performance of EPA and State programs.

CONCLUSION

With continued innovation by States, and better guidance from EPA, we hope to improve State monitoring programs and thereby improve the quality of EPA and State decision making.

INITIATION OF A NATIONAL WATER QUALITY NETWORK FOR NEW ZEALAND

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ABSTRACT

A nation-wide network for the long term assessment of water quality in New Zealand rivers and lakes has been designed and is now being implemented. The objectives of the network are to detect significant trends in water quality and to develop better understandings of the nature of the water resources and hence to better assist their management. The design has been based on the requirement to be able to detect trends within five years with good statistical power, if such trends exist. Both "baseline" (relatively unimpacted) and "impact" stations have been selected. There are 30 baseline river stations and 17 baseline lake stations. The total network includes 77 river sites and 30 lakes. River sites are being sampled monthly. Most lakes will be sampled bimonthly. There are manifold criteria for choice of variables to be measured, but these have mostly to do with their impact on water use.

In operating the network we have built a general water quality database manager, AQUAL, which will ensure that the network data are fully documented and widely available. Field and laboratory data quality assurance are being rigorously attended to. Statistical tests to be applied to the data have been proposed: indeed the sampling frequency selection has been based on the requirement to attain good detection power with such tests. There will be annual reports to government increasing in complexity up to about five years after network initiation.

INTRODUCTION

The two main islands of New Zealand - 47°S; 166°E - 179°E, surface area = 26 km^2, population about 3.2 million) h: mountainous elongated character, and : the path of wet westerly winds fron Tasman Sea. Average rainfall and run about 1500 mm and 47.5 l/s/km^2, but the: distributed rather unevenly, being larg: the west coasts. Rivers are typically st than those in continental countries. The a number of large inland lakes. The ecc is still dominated by agricultural produ sheep, dairy and cattle farming, and horticulture. These operations have (the majority of water quality problems from point and distributed sources: dis oxygen deficits, sewage fungus patche: lake eutrophication. Problems associate industry tend to be located in waters ne main cities. Most of these cities ar: estuaries and coasts.

In mid-1988 the Water Quality received funding to design a network for and streams. This built on a previou design, for rivers and lakes (McBride Research on study techniques was nc sidered to be well enough advanced tc estuaries, coasts and groundwater.

Table 1 lists the tasks which hav: considered in the design, all of whi receive attention here. Full details ar found in Smith et al. (1989).

Table 1. Tasks to be addressed

1. Develop the goal and objectives
2. Produce list of sampling sites
3. Confirm statistical design criteria, especially sampling frequency
4. Produce a list of determinands
5. Assess accuracy requirements
6. Confirm laboratory analysis procedures
7. Recommend appropriate laboratories
8. Recommend field operators and training requirements
9. Develop field sampling/analysis procedures
10. Develop procedures for sample preservation/transport to laboratory
11. Develop sampling routes
12. Develop quality assurance procedures (from bottle washing to data entry
13. Recommend data storage/retrieval/management system
14. Recommend data analysis procedures and software
15. Recommend reporting procedures (what, to whom, by whom, when)
16. Assess cost

GOAL AND OBJECTIVES

The **goal** of the network is: to provide scientifically defensible information on the important physical, chemical, and biological characteristics of a selection of the nation's river and lake waters as a basis for advising the Minster of Science and other ministers of the crown of the trends and status of these waters.

The **objectives** are to establish a national water quality database such that we can:

1. Detèct significant trends in water quality

2. Develop better understandings of the nature of the water resources and hence to better assist their management.

With respect to the first objective, the intention is to be able to detect a monotonic trend equal to the standard deviation of the detrended data over a five year period, if such a trend occurs.

SAMPLING SITES

RIVERS

There are two types of station, "Baseline" (where there is likely to be no or little effect

of diffuse or point source pollution and which will account for natural or near-natural effects and trends) and "Impact" (which are downstream of present, and possible future, areas of agriculture, afforestation, industry and urbanization). Preferably both types are required to properly address trends but in some instances only baseline or impact stations are possible. The requirements for station selection are that they should be:

a) at or close to a current hydrological recording station,

b) accessible,

c) at such a location so that transport of samples to the laboratory presents, no time constraints,

d) safe for operators,

e) free from disturbing influences such as weirs and weedbeds,

f) easy to sample and carry out *in situ* work,

g) free from saline intrusions,

h) in some way of national, multiregional or scientific importance.

Most sampling sites have been visited by the designers. Sites have been selected so that a single surface grab sample will be representative of the bulk water flowing past. Two sites only require homogeneity checking; this is being attended to. In all, there are 77 river sites, 44 in the North Island and 33 in the South Island (Fig.1). The inclusion of each site has been clearly justified.

The work on rivers commenced in January of this year.

LAKES

Lakes have been selected in two classes - the first with excellent water (pristine or near pristine) whose primary use is recreation and aesthetics, the second with eutrophication problems. In both lake classes lake selection is because of national or multiregional importance, uniqueness, or representativeness; in some instances selection is because of a perceived study value. In the first class, lakes are also selected for protection reasons.

In all, 30 lakes have been selected (Fig.1) and each clearly justified. With just one exception, a single location (normally the deepest point) has been selected for investigation through time bearing in mind that complete characterisation of each lake is not the intention.

A separate strategy has been designed for each lake. For some, surface water sampling is required, for others depth averaged sampling is required. For most lakes dissolved oxygen/temperature profiling is required, whereas for others (those which do not stratify) single sub-surface values only are to be determined.

Funding for the study of lakes has not yet been clarified and field work is not expected to commence this year.

STATISTICAL DESIGN CRITERIA

The design requirements which include the analysis of data are discussed briefly in a later section. Here we will briefly examine the statistical reasoning behind the choice of

sampling frequency for the most imp(objective, that of trend detection.

When trends in data are sought, it m recognised that there is no point in ca out short-term intensive sampling, becau effects of seasonality, extreme events, uniform variance, and autocorrelation m accounted for (Lettenmaier 1976, 1978; and Ward 1980). The practical conseq is (Lettenmaier et al. 1982, pp. 62-63) is generally difficult to detect a trend (order of the water quality variable's st deviation for n smaller than 50-100. because of autocorrelation, the mir effective sampling interval is on the or two weeks: for rivers monthly samp often optimum; for lakes, even longer. a trend to be detected, **the network mu fixed for at least five years.** This fin(strengthened by Hirsch and Slack (19: the United States Geological Survey (l in their examination of a robust nonpare trend test: reasonable power for detection for rivers may only be att; after five years of sampling. Indeed it after ten or so years of routine rive collection that the USGS is publishing of trend assessments (Smith and Ale 1983, Smith et al. 1987). Lettenmaie (1982) go so far as to conclude that re of the network should not take place ar because this encourages fragmentation data, which compromises its utility fo detection. Analysis of results of the r should be performed annually howe look for any evidence of trends en Provision of such analysis software wit proposed data management system (se is thus desirable.

The technique here is basicall promoted by Lettenmaier (1976, 197? pose the simple null hypothesis:

$$H_0 : \Delta\mu = 0$$

where $\Delta\mu$ is the change in the mean water quality variable, against the co alternative hypothesis

$$H_A : \Delta\mu \neq 0$$

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Fig 1 Sampling sites. River sites are marked with a bar and coded, lakes are named.

Because H_A is composite, the power of a test to choose between (1) and (2) is a function of $\Delta\mu$. We consider $\Delta\mu$ to be monotonic: either a step or a linear trend (higher order monotonic polynomial trends are also possible in this technique).

Our method of approach is to calculate the detection threshold ($\Delta\mu/s$, where s is the detrended standard deviation) of a test for given Type I and Type II error risks, trend type, autocorrelation, sampling frequency and length of record. Thresholds have been calculated for a given combination of α (the probability of committing the Type I error of falsely detecting a monotonic trend), β (the probability of committing the Type II error of failing to detect a monotonic trend), r(1) (the daily lag 1 autocorrelation coefficient), and sampling frequencies over 5 and 10 year periods. We have also examined autocorrelation coefficients for a variety of determinands measured during long term studies (McBride 1987).

Our conclusion from this is that an appropriate sampling frequency for linear trend detection, is monthly for rivers and bimonthly for lakes to obtain the desired detection threshold (of around unity) within a 5 year period with reasonable power ($\beta \approx 0.1$).

DETERMINANDS

All determinands have been carefully selected and included only if there are very good reasons for doing so. The temptation to include "nice-to-do" determinands has been avoided. Table 2 contains the selected determinands, where they are to be measured, whether they are for rivers or lakes, and the reason for inclusion of each.

ACCURACY REQUIREMENTS

The network has been designed to give good trend detectability for regular sampling over 5 - 10 years. The magnitude of the trend to be detected,either gradual or abrupt, is measured by the difference in expected values of observations near the start of the trend assessment period and those near the end of that period. We want this minimum detectable trend to be

as small as possible, minimising the impact of analytical and sampling errors. We cannot however, design for the magnitude of the trend on its own: we have to design for the minimum detectable trend as a proportion of the standard deviation of the detrended data And this standard deviation contains a component attributable to the unavoidable presence of errors, both analytical and sampling So the larger the error standard deviation, the larger the minimum detectable trend. Because we want this trend to be as small as possible a way has been found to: (a) calculate the effect of errors on the minimum detectable trend, and (b) indicate to the analysts and samplers what sort of performance is required

The details of how this is done are given elsewhere (Smith et al., 1989). The essential idea is to compare an attainable error standard deviation with a maximum permissible error standard deviation. If the former error is the smaller, then the trend can detected with the required power. The analysis is based on the assumption that we can ignore the effect of bias (because trend detection involves differences of means, and so most if not all bias will cancel out Hence the analysis considers only precision and considers laboratory precisions based many years of analytical quality assurance studies and anticipated field precisions based on best judgement where actual values are not available.

The upshot of this part of the design that we are in an *a priori* position to state the actual trend detectability for a variety determinands and certain concentrations values), given certain values for a and b allowing certain permissible increases detectable trend caused by errors.

To ensure that laboratories are producing accurate results, collaborative tests among them are necessary. This is to be carried out at regular intervals between the two laboratories selected for the network. It is also necessary to ensure that field analysis produces accurate results and that field sampling does not introduce inaccuracy. A comprehensive data quality assurance programme called for and has been built into the design (see later).

Table 2 List of determinands

Determinand	Where measured (field/base/laboratory)	Rivers/ lakes	Reason for Inclusion
Dissolved oxygen	f	R/L	Numerical standard; necessary requirement for aquatic life; rapid indicator of organic pollution; indicator of lake trophic state.
pH	f/b/l*	R/L	Numerical standard; aquatic life protection; pollution indicator: acidification.
Conductivity	l	R/L	Simple surrogate for total inorganic ions (incl. hardness).
Temperature	f	R/L	Numerical standard; DO interpretation; mixing in lakes: aquatic life protection.
Visual clarity (black disc); Secchi disc depth	f f	R (initially†) L	Descriptive standard: visual monitor; erosion/habitat destruction; aquatic life protection (clarity only); public perception.
Turbidity and absorption coefficients	l	R/L	Descriptive standard. Turbidity as support to on-site clarity measurement, absorption coefficients relate to water colour, light climate for plants and organic character of water.
BOD$_5$	l	R	Descriptive standard; organic pollution indicator.
Dissolved nutrients: NH$_3$/NO$_3$/DRP	l	R	NH$_3$ is proposed numerical standard for potable supply; NO$_3$ required for public health issues; enrichment potential for algal growth.
TP/TN	l	R/L	Nutrient status/eutrophication.
Flow	f	R	Flow dependence analysis.
Lake height	f	L	Height dependence analysis.
Chlorophyll a	l	L	Descriptive standard: possible water use change indicator; nutrient status indicator.
Benthic invertebrates**	l	R	Descriptive standard; water use change indicator.
Nuisance periphyton growths	f	R	Descriptive standard; visual monitor; public perception
The following for first year only:			
Ca/Mg/K/Na/Cl HCO$_3$/SO$_4$	l l	R/L R/L	Major ions including hardness species; general assessment of water quality; HCO$_3$ drop and SO$_4$ rise indicators of lake acidification.

NOTES:

1 The term 'standards' refers to the current and proposed standards.
2 The 'first year only' ions should be measured at a later stage only if conductivity appears to be changing. There is one exception to this; for lakes it may be wise to measure HCO$_3$ and SO$_4$ in each sample as a reassurance that lakes are not being acidified.
3 No bacterial measurements are recommended at present. Faecal coliforms are stipulated in legislation but the wisdom of this is being seriously questioned. For instance EPA (1986) recommend E. coli and enterococci for freshwater bathing criteria. In addition there are problems with sampling frequency differences between legislation and what is practical for a national network. There are also difficulties with interpretation. We should await results of research before embarking on a costly analysis which is of dubious value.

* pH will be measured in the field, back at survey base, and in the laboratory (as an additional check) for the first year. If, after this period, there is no difference between field and survey base measurements, field measurement may be discontinued. This decision must be made with caution.

** Benthic invertebrates can be collected at about 70 of the proposed river sites and data will be analysed for changes in community composition and species abundance.

† Black disc measurements will be made initially only on rivers. When current research is complete, a recommended method for horizontal black disc distance in lakes will be available. Both vertical and horizontal measurements will then be made.

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LABORATORY ANALYSIS PROCEDURES

To ensure that both laboratories treat and analyse the samples in an identical way, sample processing flow sheets have been drawn up and a list of preferred analytical methods established. The flow sheet for riverine samples is presented in Fig. 2.

LABORATORIES AND FIELD OPERATORS: TRAINING REQUIREMENTS

Several studies have shown the difficulties associated with the use of a multitude of different agencies for a national water quality network. For instance in the UK, Fenlon and Young (1982) noted that the harmonization of results (i.e., the production of results of known and adequate accuracy), which is difficult on the regional scale, has proved to be even more so at the national level and had been achieved to only a limited degree seven years after the inception of the UK Harmonized Monitoring scheme. In addition, there is also no harmonization in the manner in which data are supplied to the central data repository, the Department of the Environment, in large part because there are 16 autonomous contributing agencies.

In the USA, the General Accounting Office has stated that "inconsistency in field work and laboratory performance make it virtually impossible to meaningfully compare network data from month to month, season to season, and year to year" (GAO, 1981).

Consequently a single agency (the DSIR's Water Resources Survey field party network) has been assigned the task of field work (i.e., water sampling and field analysis [which has been kept to a bare minimum]), and just two laboratories have been selected for the laboratory analysis (one in each island). Samples taken in each island are analysed in the respective laboratory. This ensures that samples arrive at the laboratories overnight, a sample preservation requirement (samples are chilled under ice after collection and must remain so until they are processed). It is possible that other organizations could join the Network later, if the necessary standards are attained.

The training requirements of field sta been addressed by recently holding a r training course to supplement previous and video training films. At the emphasis was placed on correct procedures for ensuring: accurate and measurements are obtained for d oxygen concentration, pH, and temp contamination-free water sampling ai sampling; benthic invertebrate samplin consequence of the course modificatio been built into the recommended meth instance, insistence on the use of ca thermometers to check field probes easily overlooked), the use of known concentration sodium bicarbonate s (equilibrated with atmospheric C(simulate natural waters as a check functioning of pH probes (this is in adc the normal calibration procedure wl itself is inadequate when dealing with buffered, low ionic strength natura samples). Without such checks little can be placed on the reliability of resu the apparently simple task of temperature and pH measurements.

SAMPLING ROUTES AND SAMI PRESERVATION/TRANSPOR1

Once the sampling sites had beer lished, each of the 15 field parties wa to consider an appropriate sampling i ensure that each river site was vi approximately the same time of day visit and that site visitation was key their already established work load (i. hydrological station visits/maintenanc this stage it was stressed that it was j better to avoid doing the water quali as an add-on to their normal work loa it was certain that the additional ef not likely to compromise the water work.

It is important that samples can b ported overnight to the laboratory sample preservation is achieved si chilling under ice in an insulated b overnight commercial land courier se been built into each sampling route t this occurs. Use of airlines has been
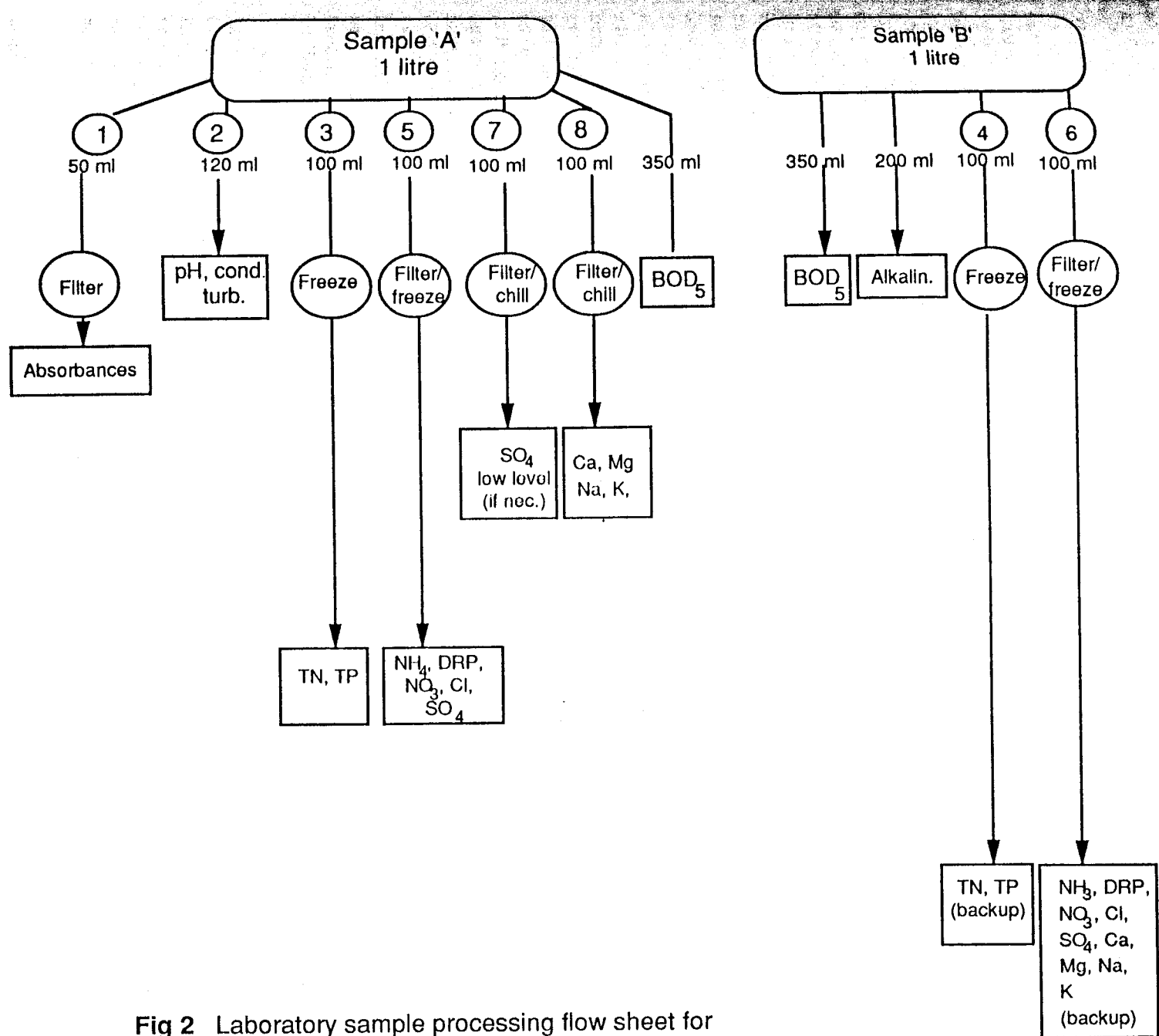
Fig 2 Laboratory sample processing flow sheet for rivers.

FIELD SAMPLING AND ANALYSIS PROCEDURES

RIVERS

The location of each sampling site has been specified. The requirements for each site have been spelt out to field parties and reinforced by carefully thought out field sheets (see Fig. 3 for an example) which must be filled in at the time. The design of the field sheets has been carried out with the cooperation of the field parties - indeed the cooperation of, and input from, field parties has been sought at all appropriate stages in the network design. This was felt to be important.

At each site, each month, a bulk representative water sample is collected in a large, clean container and this is then subsampled to meet the sample requirements of the laboratories. Additionally, a small sample is collected for measurement of pH back at field party base (in the first year of the network pH is being measured in the field, back at base, and the following day in the more controlled conditions of a well-appointed laboratory to establish what happens to pH during time). Dissolved oxygen and temperature are also determined in the field. Water clarity is determined using a specially constructed black disc viewed horizontally (Davies-Colley, 1988). This provides a more appropriate measure of clarity than the conventional Secchi disc depth because it relates better to the sighting range of riverine animals, gives a measure of the beam attenuation coefficient, and finally it can actually be measured in a shallow river. Finally an assessment is made of nuisance periphyton cover.

Each year an appropriate number of samples are taken of benthic invertebrates.

For all the above requirements, detailed instructions have been sent to field parties

LAKES

The requirements for each lake are specific to that lake and only the main features can be addressed here. With one exception (Lake Rotoiti, North Island - and this behaves almost like two lakes because of its shape, one

of which is somewhat polluted) wor conducted at a single site. This specified precisely and marked on metric chart (available for all but tw

Most lakes are to be visited e months, others whose dissolved oxy centration may drop rapidly in summe at least monthly visits during this p dissolved oxygen profiling. This is information on depletion rates car tained. As for rivers, a bulk samp quired; in some cases this is taken below the surface whereas for the ma samples are required from a series and these are mixed. For the latte spaced samples are to be taken rou the photic zone - how to estimate the Secchi disc depth has been calcula published relationships and water refl and a list of multipliers will be furr field parties. For clear and/or relativ lakes the photic depth may be gre the mixed depth for a period in mid in which case sampling is to be ca over the mixed depth to avoid possible layers of detritus which associated with the thermocline. In and to avoid possibly sampling too biasing the bulk sample, the actual r sampling depth has arbitrarily been se of the photic or mixed depth, whiche smaller. A carefully detailed proce been developed for the field parti above, after all, is rather complex and field estimation of the mixed depth, easy task.

The bulk sample is to be subsample laboratory analyses and an additio litres taken for filtration for su chlorophyll *a* analysis. For the l estimate of the volume required i obtained from the Secchi disc depth lakes; again explicit instructions provided.

Field pH is to be measured on the of the bulk sample and a further s taken for pH measurement back at for rivers). Dissolved oxygen and tem are to be measured just below the su those few lake for which profiling propriate (i.e., very shallow, well mixe

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(This sheet must accompany samples dispatched to the
laboratory for analysis - one sheet per site per visit)

Day.............................. Date............................... Field party area...............

Field operators' names ....Time (NZST):

Site code: Site Description: Cloud (/8):

Gauge ht (m) (external):   (internal):   Flow (m^3/s):

Water temp ($^\circ$C) (corrected):   DO (% satn):   Atmos.press. (mbar)($\pm$5)

Black disc dist (m): (a)   pH (field):   pH (base):
(2 observers) (b)   8.28 check: 8.28 check:

	Obs.	1	2	3	4	5	6	7	8	9	10
% peri- phyton cover	Filament -ous										
	Mats (>2 mm thick)										

Periphyton colour (filamentous):   (mats):
Observation site (circle one): open/shaded
Comments:

Notes:

1   At each site measure and record temperature, pH, DO and horizontal black disc distance. At end of day re-measure pH on samples collected in 120 ml containers. Also, obtain and record values for gauge ht, flow and atmospheric pressure.

2   At each site fill two 1 litre plastic containers and one 120 ml container. Cap tightly, leaving no air space if possible.

3   Assess % periphyton cover at 10 equidistant points across the wadeable area of a 'run' near the water sampling site. Improvise as necessary to get 10 observations.

4   Comments could concern: exceptional low/high flow conditions and antecedent weather; surface scums, foams, oils and slicks; anything unusual, e.g. different or unusual colour.

Fig 3 Field sheet for rivers.

In addition the Secchi disc depth is required; when research is complete on the logistics of measuring the horizontal black disc range, this plus the vertical black disc depth (analogous to Secchi disc depth) will be required.

QUALITY ASSURANCE PROCEDURES

Here we are referring to all aspects of ensuring that measurements made in the field and laboratory are within accuracy specifications, and that transposition of data and loading onto computer files occurs without error.

For field measurements, quality assurance procedures have been built into each method, and each sampling bottle has been coded and is dedicated to a particular site.

The two laboratories are expected to maintain normal quality assurance procedures, i.e., by using appropriate blanks and known solutions, and production of control charts as appropriate. In addition, test solutions (these can be either complete unknowns or known solutions) will be periodically sent to each laboratory for analysis. Even the techniques for routine bottle washing have been provided for use by the laboratories.

Built into the data processing package (AQUAL) is a checking system to ensure that all results entered could be reasonably expected for New Zealand's fresh, surface waters. In addition, prior to data entry they are sighted by an experienced technician who looks for oddities.

DATA MANAGEMENT SYSTEM AND ANALYSIS OF DATA

DATA MANAGEMENT

There is a dearth of water quality data archive software available. As a result, data documentation and availability are often compromised badly - meaning that the information content of the data is not extracted. It may not even be known that data exist. We have attempted to avoid this problem in New Zealand by producing a water quality database program: AQUAL (AQuatic Unified Archival Library).

This program enables users to interpret, retrieve and exchange water q data. It has been designed to do so in that makes using the program as easy a flexible as possible. At the same tir ensures that sufficient information is giv that data are stored and retr unambiguously. The user interface consi menus of options, full-screen data entry prompts. Entry into some screen fie mandatory - to avoid ambiguity problen an input error is made, the user is pror with a helpful error message. Default e appear in appropriate fields automaticall can be overwritten.

In using AQUAL, the sites, ana methods, and project must first have "registered". In registering a site it is as an identifier that is used in subsequent r sample data entry. The type of site river,...) must be given along with appropriate data. In registering an att a nickname is assigned, as well as the code that the sample data values are at to in the database. Use of the nicl which can be changed if a new an method is adopted, greatly simplifies quent routine sample data entry. The that the attribute values are to be stc must be defined. A minimum and ma can be defined for each attribute: if bounds are exceeded when sample d entered a warning message is posted screen. A comment can, and shou entered with each attribute registrat least the definition of what the analyst by "detection limit" should be stated he registering the project (i.e., the N Water Quality Network), an identifier list of attributes to be measured are as

Registration of sites, attributes, and are all done in a password-protected se the program. In this section sample d also be "verified": data entered into A are considered to be unverified until leged user (i.e., one who knows the pa changes it to "verified". The only otl tion of AQUAL that is password prot where bulk data are imported to the d

The routine use of a data arc running a network is to enter samp

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such as a DO value. This is done in the Sample Data Entry section. There are two steps: *sample registration*, and *sample data entry*.

In other sections data can be selected by a variety of logical criteria, the selected data checked, and reports made on it. Such reports can be for verified data only, for unverified data only, or for both types of data. Of particular note is that user-defined reports can be made on combinations of the selected data, with full summary statistics (accounting, nevertheless, for "less than", "greater than" and missing data). These also give stem-leaf diagrams (numerical histograms) and two normality normality tests. Linear regression tables (appropriate if the normality tests do not indicate strong skewness in the data), correlation matrices, and simple data plots can be obtained. Bulk data can be transferred inward or outward via formatted ASCII files that the user can prepare. This feature can be used to export data to a statistics package to perform more complex statistical analyses.

DATA ANALYSIS

Any data analysis protocol must contain three elements (Ward *et al.*, 1988): (a) procedures to prepare a raw data record for statistical analysis; (b) means to display the behaviour of the water quality variables over time, for trend analysis; (c) recommended statistical analysis procedures to provide the desired information.

In the case of the National Water Quality Network, these three elements are fused into two parts:

(i) regular checks within each year for consistency, errors, and outliers;

(ii) yearly reports of the features of the data to date, including emerging trends.

Part (i) includes all of element (a) and some of (b) - the display of the raw data. Part (ii) covers all of element (c) and the rest of element (b) - the display of data interpreted using the (c) procedures.

Note that these yearly reports will become more substantial as time goes by, because trend detection power will increase with the length of record.

Part (i): regular within-year checks. This can all be carried out using AQUAL. In particular, the summary statistics and stem-leaf diagrams in AQUAL should be used. These will show up any outliers. If appropriate a plot of the attribute value versus time could be obtained also.

Part (ii): annual reports. The main features of Network data, excluding trend analysis, can be obtained from the data checking and user-defined report AQUAL options. We expect that heavy use will be made of the summary statistics feature of the user defined report in this.

For trend analysis, we are recommending following mostly the data analysis procedure used by the USGS (Crawford *et al.* 1983). This procedure is well written and has been used successfully to report on trends in their NASQAN and NWQSS networks (Smith *et al.* 1987).

The analysis will be based on the following sequential steps:

1. Compute flow adjusted data (river sites only);

2. Visually inspect the raw and any flow adjusted data for each site;

3. Perform appropriate nonparametric statistical tests, indicated by the visual inspection, on the raw data and on any flow adjusted concentration (FAC) data.

In performing trend tests, nonparametric procedures offer the following advantages (e.g., Lettenmaier *et al.* 1982, Hirsch *et al.* 1982, Helsel 1987, Ward *et al.* 1988):

- they are always valid, whatever the distribution of data happen to be;

- they are nearly as powerful as parametric tests when the assumptions of such tests

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DEVELOPMENT OF A WATER QUALITY MONITORING SYSTEM IN QUEENSLAND

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ABSTRACT

The development of Queensland depends on the availability of both surface water and groundwater. The assessment of these resources both in quality and quantity is the responsibility of the Water Resources Commission. In the past, the emphasis has been placed on assesing quantity, but recently a concerted effort has been directed to evaluating their **quality**. This paper looks briefly at water resources development and the causes of water quality problems in Queensland. The present water quality monitoring network and its inadequacies are described; methods of evaluating data are extensively discussed and results provided, and the principles of the design of a water quality monitoring network for Queensland are given in a case study of the Upper Condamine River basin.

INTRODUCTION

Queensland is the second largest state in Australia. Its area of 1.7 million sq. km is roughly 23% of the total Australian land mass. The population is 2.5 million and is concentrated in the south eastern corner and at major towns along the eastern coast. The remaining 21% of the population is scattered throughout western and far northern areas. The most prominent land feature is the Great Dividing Range which separates the relatively steep, narrow coastal fringe from the flat, dry interior.

Water quality problems are generally associated with the closely settled areas of the south east and the coast. The main sources of pollution are from agricultural land use.

The rise in soil salinity resulting from clearing forests, the subsequent rise of groundwater, and excessive soil erosion due to inappropriate land management, are the main causes of deterioration of water quality in agricultural areas. In some areas, sea water intrusion into coastal aquifers, resulting from depletion of the groundwater resource, is a potential threat to irrigated sugarcane, orchards and small crops.

In Queensland, water quality problems are exacerbated by climatic extremes. Rainfall is not only highly seasonal, it is also extremely variable. Long droughts of 12 months or more may be followed by tropical cyclones or rain depressions which can commonly result in 200 to 300 mm of rain in one or two days; some 800 mm was recorded in one town on March 1, 1988. Such cyclonic rainfall events may well be one quarter or one third of mean annual rainfall. Fertiliser-rich soils washed out by the resulting floods can have a major impact on the rivers and streams in which they are deposited.

Well-planned water quality monitoring has become a necessity because the rapidly expanding urban and agricultural development of the state is putting an increasing burden on the limited natural water resource in ways that cannot be foretold from past experience. Early warning of the potential hazards would prevent serious economic losses, especially in times of weather extremes. Added to this is the opportunity to make full use of the

resource by being able to predict with confidence the volumes of good quality water which can be made available to consumers.

In Australia the state authorities monitor and control water quality in streams and storages.

Water Quality is regulated in Queensland by three acts:

1. Clean Waters Act 1971-1988;
2. Water Act 1926-1987;
3. Water Resources Administration Act 1978-1989.

The last two acts are administered by the Water Resources Commission which is the state authority responsible for the development and management of water resources in Queensland. Under the relevant provision of the Water Resources Administration Act the Commission is responsible for keeping records of the natural water resources in the state. It

is also responsible for assessment of the available water resources and their protection.

The responsibility for the investigation and prevention of pollution and the issue of licences controlling the discharge of effluent into receiving waters is with the Queensland Department of Environment and Conservation.

The Water Resources Commission's responsibility for development and management of surface waters extends only to the tidal limit. However, no similar specific demarcation line is drawn regarding groundwater and accordingly the Commission has a responsibility to deal with problems of salt water intrusion in coastal aquifers.

EXISTING NETWORKS

The Commission has established several monitoring networks throughout the state in fulfilling its role of assessing and managing water resources. These are:

NETWORK	No. of STATIONS
water quality	. . . 2900
stream gauging	. . . 400
groundwater level:	
- artesian	. . . 180
- sub-artesian	. . . 5000

It has been the practice of the Commission to sample surface water at stream gauging stations during visits by hydrographers, and at specific sites on streams by licensing officers. Because of the strongly seasonal and extremely variable rainfall conditions in Queensland these visits normally coincide with periods of low or medium flow. There are, however, some samples taken during flood events. The

network was designed in the 1960's and had as many as 700 stations. However, it has recently been the subject of an extensive review and currently consists of approximately 400 stations. The major physical and chemical parameters such as conductivity, pH, dissolved ions, dissolved and suspended solids, hardness, alkalinity, turbidity and sixteen major ions are currently analyzed in the laboratory.

The situation is similar in regard to the sampling and analysis of groundwater. There are some 2500 bores sampled in Queensland. At many of them only conductivity is measured as a general indicator of water quality. A similar range of analyses to that for surface water is performed for other bores. The frequency of sampling varies, but most of the bores are sampled at least once a year.

Until recently little attempt was made to analyze the water quality data to determine their accuracy, to assess whether they were representative of the source and whether the techniques being used were relevant or appropriate. Data were extracted for a limited area whenever a project started or a basin resource was to be re-evaluated.

In 1988 a decision was made to re-design water quality monitoring networks and information systems which would reflect the future needs of the water industry in the state.

The main objectives of the groundwater and surface water quality monitoring network are:

1. To determine the spatial and temporal variation of water quality throughout the state.

2. To determine the suitability of the waters for urban, industrial, agricultural, private and general community use.

3. To provide a set of benchmark stations to assess future changes, especially the effects of changes in land use.

4. To estimate mass transport of several water quality parameters.

5. To determine sources of variation in water quality as a tool for understanding and predicting water quality and quantity.

METHODS FOR EVALUATING DATA

GENERAL

The Water Resources Commission has acquired thousands of individual analyses of natural waters dating back to the 1940's. Unfortunately, prior to about 1970, many of the samples were collected using less than ideal methods. Unsuitable containers such as unwashed drink bottles were sometimes used to collect samples, and it was not unknown for a sample to be decanted or filtered before delivery to the laboratory. Also, due to limited laboratory facilities, analysis of samples was often delayed, sometimes by as much as eighteen months.

In order to design a monitoring network for maximum efficiency, it is necessary to use as much of the information on water quality in the area as possible, so that the most sensitive monitoring sites can be selected and the most suitable sampling times chosen to allow for normal seasonal variation as well as long-term trends. The Commission's existing bank of data provides both long-term information and a wide coverage of the natural waters, so that if the accuracy and reliability of the individual analyses could be determined, the acceptable data could be used to map out a seasonal and spatial statistical picture of the water quality, saving the enormous costs of fresh field surveys.

Reliability of Existing data This was done by comparing this data with data from the Department of Local Government. The latter data were independently collected by that Department since the 1940's in order to establish and monitor town water supplies. Hence, considerable care was taken in the sampling and analysis techniques used. Where these analyses are available, they are being used to build statistical portraits of the many natural waters encountered in the state, taking into account such factors as region, season, depth of bores or discharge of streams. This gives a standard for distinguishing aberrations from normal variability in the much more extensive water quality data base acquired by the Commission.

The statistical software package SYSTAT v.4 with SYGRAPH was selected to explore and compare the two data sources. Initially, a pilot study was carried out on the Upper Condamine River basin in the south-east of the state (Fig. 1). This is the first region to be included in the new monitoring network.

FIGURE I

LEGEND

— · Catchment Boundary

▲ Stream Gauging Station

· Bore Location

UPPER CONDAMINE VALLEY
WATER QUALITY MONITORING
SUB-AREAS
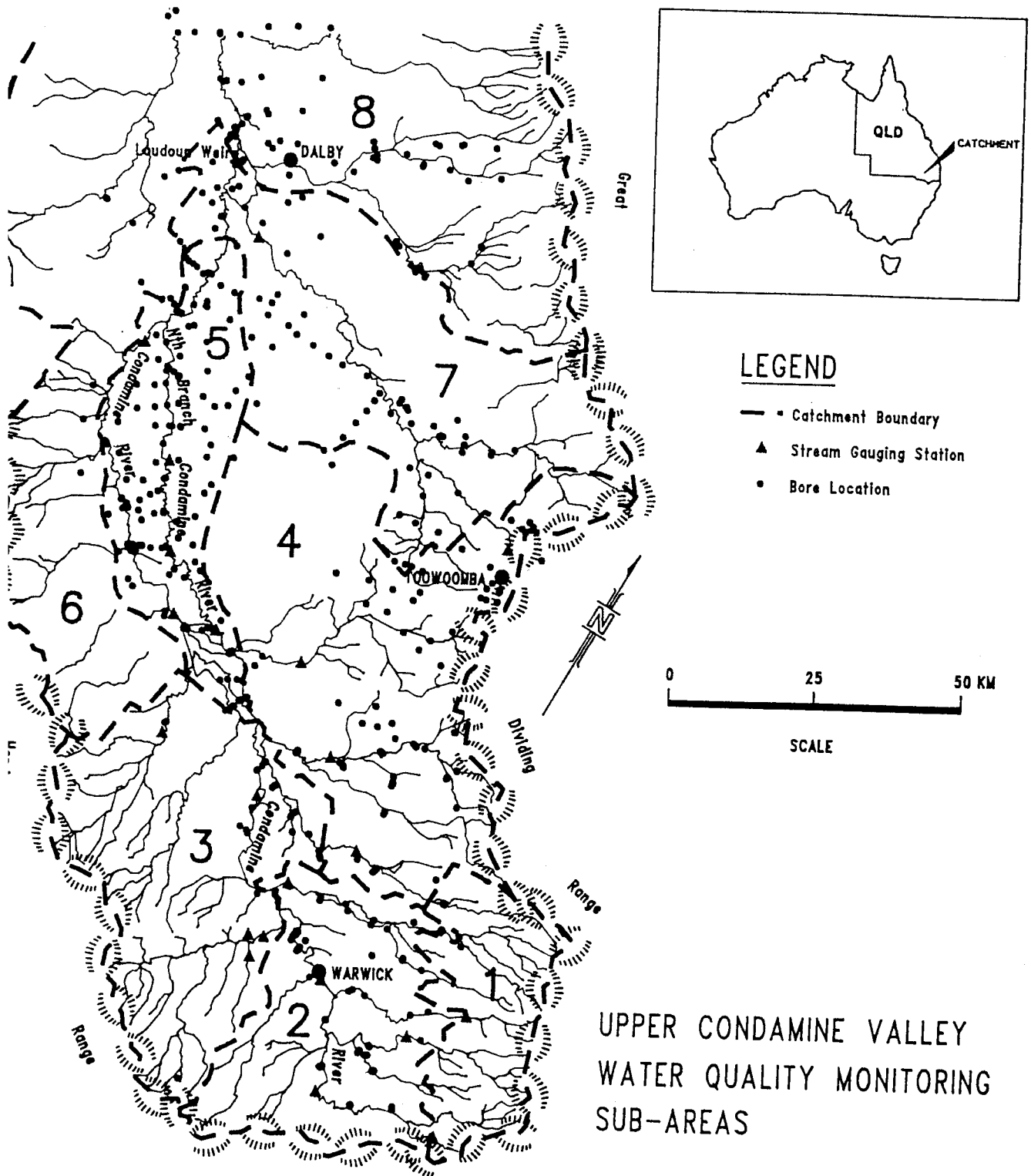
Analyses taken from the 1940's to the 1970's from Loudoun Weir, which is the exit point of the region and the water supply for the town of Dalby, provided a sample set on which to test the suitability of the procedures available in SYSTAT.

The list of variables used initially for processing with SYSTAT included the date of collection, conductivity where available, "total equivalents" (mean of cation and anion milliequivalents per litre), and the percentage equivalents of the major ions: sodium, potassium, calcium, magnesium, chloride, sulphate, carbonate, bicarbonate and nitrate. Other ions such as fluoride, phosphate and iron occurred only as traces, or were not consistently analyzed for, or were recorded in various forms. These were treated separately.

PRELIMINARY TESTS:
A series of tests were carried out on the whole set of town water supply data for Loudoun Weir. There were sixty-one analyses, sampled between the 1940's and 1970's, but most consistently during the 1950's. Gauge heights (river stage) were not available for most of the period of record, but in most instances a description of stream conditions was made at the time of sample collection. There are many reliable long term rainfall stations covering the Upper Condamine Basin.

The procedure of the tests was as follows:

Firstly, a histogram was plotted (Figure 2), showing how much the samples depart from perfect ionic balance: (Total Cations - Total Anions)/(Total Cations + Total Anions) as a percentage in milliequiv./l .

This graph covers all surface water samples from the Condamine. The large peak at zero is explained by the fact that many earlier analyses were computed assuming perfect balance. The range illustrated suggests that a discrepancy of greater than five percent should be questioned.

Secondly, conductivity was plotted against Total Salts. Curves were plotted to determine how much departure from the norm would be an acceptable range of variability.
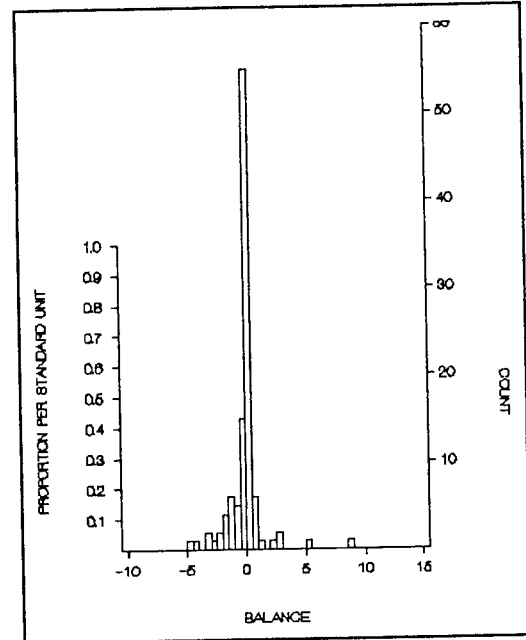
Figure 2 Histogram of ionic imbalance.

Thirdly, the cation and anion totals were computed and compared with those given with the analyses.

These three tests should be sufficient to diagnose significant arithmetical or typing errors in the major ions.

MULTIVARIATE METHODS
In a basin the main influences on water quality are the source of the water and the climate. The next step was to submit data to classification procedures, such as Cluster Analysis and Factor Analysis so that the 'types' of water, seasonality and discharge could be taken into account when deciding the normal variability in TSS and proportions of the various ions.

Cluster Analysis
Cluster analysis is a multivariate procedure for detecting natural groupings in data. The approaches which we have found to be most appropriate for categorising water quality data are discussed here.

Decisions have to be made regarding the number of groups to end up with, and the method of measuring the 'distance' between

two clusters, before starting to cluster data. Rules of thumb (Williams, 1975) for the final number of groups include :

- use 6 to 10 because humans can only handle 5-9 'chunks' of data at a time;

- use the square root of the number of samples;

- use the log to base 2 of the number of samples, or

- make some sort of compromise.

For measuring distances or dissimilarities between samples, a Euclidean metric is easiest, although we have had good results in the past with the Manhattan, or "city block" metric. However, with clusters, there is the additional question of which linkage method to use, i.e. which point on each cluster to measure from. The methods we have found most useful for water quality work are the Single Linkage and K-means discussed in Hartigan (1975), the Centroid and closely related Average and Median Linkage covered by Sokal and Michener (1958) and Gower (1967), and the Complete Linkage of Johnson (1967).

Applications All of the clustering methods were used on the sixty-one town water supply samples from Loudoun Weir and the results compared. The median linkage result was chosen as the standard, and the first fourteen clusters were examined. After comparison with the other cluster analyses, some of the clusters were recombined, finally giving five clusters (Figure 3), whose members were checked against rainfall and river stage information. The results were as follows:

CLUSTER	RIVER STAGE
A	large floods
B	high flows
C	medium flow
D	first rise after dry spell
E	very sluggish or non-flowing

To examine the behaviour of the TSS and the proportions of the various ions within each cluster as well as in the sample space as

a whole, the samples, expressed as percent equivalent weights, were plotted on triangular diagrams. The vertices were 100% calcium, 100% magnesium, and 100% (sodium plus potassium) for the cations, and similarly 100% chloride, (sulphate plus nitrate), and (carbonate plus bicarbonate) for the anions. The cluster name was plotted at each point.
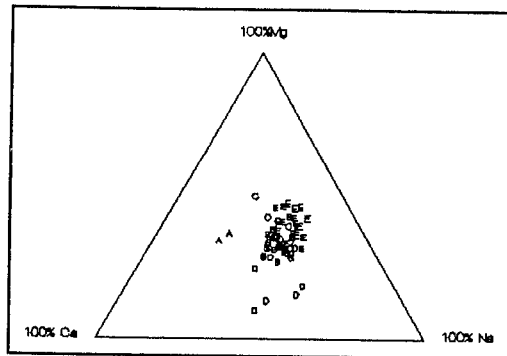
Figure 4 Cation proportions in clusters (in equivalents).

Results show (Figure 4) that the cations are well balanced, being concentrated in the middle of the diagram so that samples are seldom dominated by more than fifty percent of any one species, but that the waters of cluster E are relatively low in calcium. A likely explanation for this is that as the water level falls and the water stagnates, magnesium ions emanating from the basaltic headwaters and initially trapped on montmorillonite clays in the banks, are released by ion exchange. Another noticeable feature is the wide variability that occurs during floods, (cluster D and cluster A, which is really a group of scattered low salinity clusters put together for convenience). This is hardly surprising in such dilute waters, where local factors in the vicinity of major runoff would be crucial.

The anion triangular diagram is less interesting because nitrate and sulphate are not prominent in the region. Anion relationships are more clearly defined by plotting the anions individually against total salts (Figure 5).

This showed a strong correlation between chloride and total salts, and a less well developed negative correlation between carbonate species and total salts, with

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Figure 3

Tree diagram of cluster analysis–Loudoun Weir.

CLUSTER   RIVER STAGE

A   large floods

B   high flows

C   normal flow

D   first rise after dry spell

E   very sluggish or non-flowing
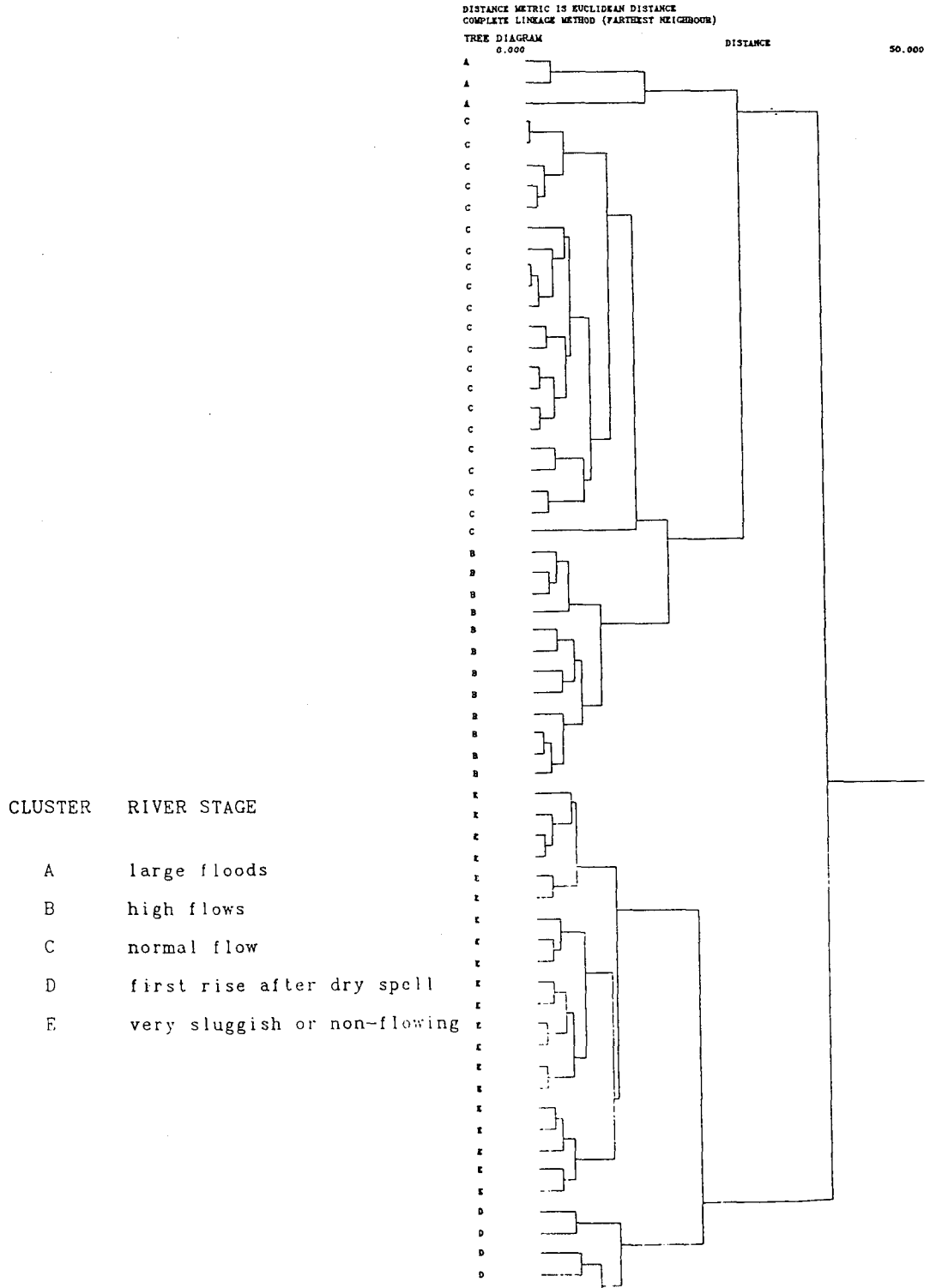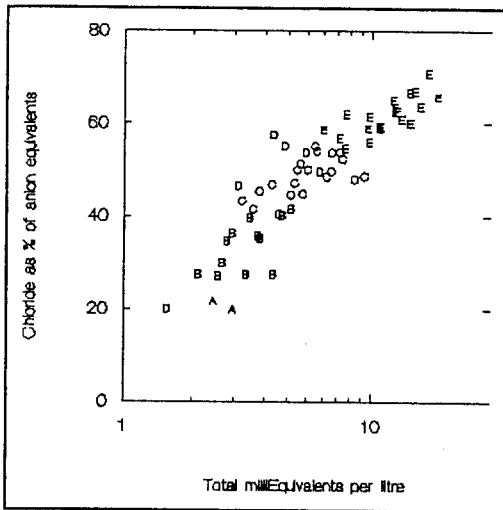
Figure 5 Proportion of Cl vs Total Equivalents.

scattering in the low salinity ranges, especially in clusters A, B, and D. A picture was thus built up of the normal variability of the water at this point under all flow regimes, and the results compared with the Water Resources Commission samples, all of which compared satisfactorily. Ground and surface water from other parts of the basin will be cross matched in the same way and the reliability estimated for all of the samples in the Water Resources Commission data base. A measure of the ability of the cluster analyses to classify water is indicated by the fact that one of the Local Government samples which refused to join a cluster, even though it was only marginally more saline than cluster E, turned out to have been collected from a bore. This sample was too closely matched in its individual components to have been differentiated from the main group by direct comparison. It was removed from the data set before the latest run.

As a further check on the reliability of samples where analysis was not done promptly after collection, volumes of water are to be collected from representative sources, subdivided and held in storage. Subsamples will be sent progressively for analysis so that the alteration of composition with storage time can be better estimated.

Factor Analysis. It is attractive to suppose that the variation evident in a population is due to a small number of underlying "factors", operating separately and each identifiable from the way the data gets "strung out" along the direction in which the process is pushing.

This is in contrast to cluster analysis, which combines actual samples into water types based on their relative similarity.

The usefulness of factor analysis is being investigating for two different purposes. The simpler use is to get a small number of independent, equally weighted variables for clustering instead of the large number of closely related ions, etc., to see whether there is any benefit in complying with the sorts of assumptions beloved of statistical theoreticians. The more ambitious use is to look for underlying processes driving the water quality occurrences.

Factor analysis (Thorndyke, 1978) regards the samples as a cluster of points plotted in multi-dimensional space, using the original individual variables (e.g. major ions in this case) as axes. It then attempts to find a new, "better" set of coordinates (axes) onto which the data can be plotted, using the following rules:

* the new descriptors are linear combinations of the original ones (e.g., $2Na - (Ca + Mg)/2$);

* there are enough new descriptors, and they are sufficiently independent of each other, to fully describe all the "important" variability in the data;

* the smallest possible number of new descriptors is used.

The SYSTAT statistics software produces an iterated principal axis factor analysis with optional orthogonal rotations. Correlations or covariances may be factored.

Typically the first factor is a vector pointing towards the most extreme of the common water types in the samples. The second factor is constructed by passing another vector through the cluster, at right angles to the

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first, which accounts for as much as possible of the remaining variance in the samples. The factors may represent a set of hypothetical water types from which all of the samples could have been derived by mixing.

It is hoped that factor analysis and cluster analysis, used with caution, may be helpful in identifying sources and zones of influence of natural waters.

TIME SERIES

The multivariate methods discussed above are used to provide a synthetic description of water quality in an area.

When information is needed on the time behaviour of a specific parameter then two methods are used:

- The seasonal Kendall-τ test (Hirsh et al, 1982)

- The Auto Regressive Integrated Moving Average (ARIMA) model (Box and Jenkins, 1976)

These methods were selected because they can handle a series of data collected at irregular intervals.

An advantage of the Kendall test is that it provides a single summary statistic figure for the entire record. However, in its simple form it does not indicate whether there are trends in opposing directions in different months.

On the other hand, the ARIMA model is used for short term forecasts. The value of these methods for Queensland conditions still needs to be fully assessed.

These methods have been applied in the Barker-Barambah catchment in South Eastern Queensland (Figure 6) to indicate possible trends of salinity. A large dam has recently been constructed in the catchment for irrigation in this agricultural area.

The salinity of Barker Creek is above that normally encountered in Queensland streams due in part to natural geological conditions of

the region and land clearing. The situation has been aggravated by the construction of a large coal-fired power plant, which discharges recirculated cooling water to a tributary of Barker Creek. Consequently, the conductivity in Barker Creek reaches 2000 uS cm^{-1} @ 25 °C with an average of the order of 1300 uS cm^{-1} during low flows. This type of water may require special management for salinity control and the salt tolerance of the plants to be irrigated must be considered.

Kendall-τ Examination of results of the seasonal Kendall-τ test is encouraging. Records of more than 20 years at five stations have been analyzed. Results are shown in Table 1.

The tabulated p values indicate that the salinity is increasing with time in Barker Creek at Wyalla/Glenmore ($p < 0.05$) and in Barambah Creek at Ban Ban ($p < 0.01$)

However, at the other sites there is no evidence to suggest such a temporal trend at the $p = 0.05$ level. (One may wish to argue that requiring 95% certainty is too rigorous a test, or indeed that conserving the status quo requires that Stonelands, for example, be treated as a developing salinity problem even if this conclusion would be wrong 20% of the time.)

Brookland and Litzows gauging stations represent relatively undeveloped and forested catchments. Here the trend S is, if anything, negative (falling salinity).

The situation changes for the remaining gauging stations. Agriculture is fairly well developed in the areas associated with them and Barker Creek is affected by releases from Tarong Power Station. Consequently the sign of S changes to positive which suggests there is a tendency towards increasing conductivity with time.

Auto Regressive Integrated Moving Average
The same data was modelled using the ARIMA model (Table 2). The 12-month forecast suggests that the mean conductivity for 1989 may be, if anything, slightly lower than the mean of the last 20-odd years, except at Ban Ban.

FIGURE 6
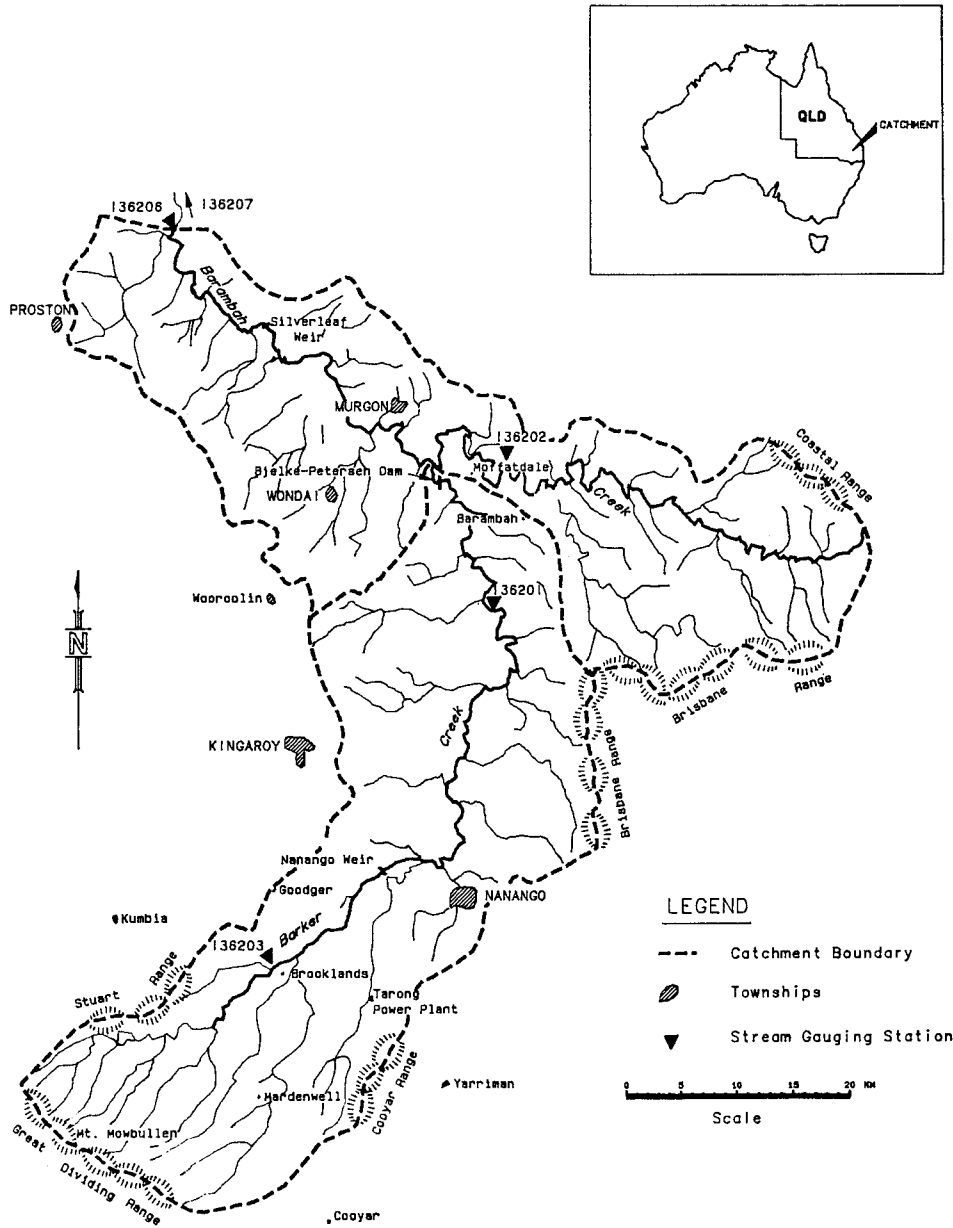
BARKER-BARAMBAH
CREEKS
LOCALITY MAP

TABLE 1. RESULTS OF SEASONAL KENDALL- TEST

Stream	Station Name	Station Number	Conductivity Statistics			
			S	B	Z	p
Barker Ck	Brooklands	136203	-17	-3.333	-0.583	0.719
Barker Ck	Wyalla/Glenmore	136201	58	14.286	1.672	0.0475
Barambah Ck	Litzows	136202	-5	-2.000	-0.116	0.5478
Barambah Ck	Stonelands	136206	28	10.001	0.895	0.184
Barambah Ck	Ban Ban	136207	72	19.915	2.713	0.0034

Note: S = Kendall trend estimator

B = Slope Estimator (in uS cm^{-1} @ $25°C$ per year)

Z = standard normal deviate representation of S

The hypothesis being tested is that salinity is increasing with time, so

p = the probability of the sample showing a non-increasing trend.

TABLE 2. RESULTS OF ARIMA MODEL

Stream	Station Name	Station Number	Conductivity(uS cm^{-1})	
			Mean of Series	Mean of Forecast
Barker Ck	Brooklands	136203	930	847
Barker Ck	Wyalla/Glenmore	136201	1288	1116
Barambah Ck	Litzows	136202	1076	1033
Barambah Ck	Stonelands	136206	1394	1365
Barambah Ck	Ban Ban	136207	1012	1028

So far, 1989 has been a wet year in Queensland, and the conductivity could be expected to be lower than the average.

Summarising, these tests seem to be useful tools for the identification of specific water quality problems. As a result of the analysis of the Barker/Barambah catchment several recommendations will be made regarding monitoring of soil erosion upstream of the storage (continuous monitoring of turbidity) and water quality monitoring in the storage. This will allow timely advice to be given to farmers and storage managers.

DESIGN OF WATER QUALITY NETWORK FOR QUEENSLAND

INTRODUCTION

The statistical methods described above are the basic tools now being used by the Commission to develop a cost effective water quality network which will meet future requirements.

Cluster analyses are being used for the determination of representative sites and intervals of sampling. It is intended to select sites in which clusters representing particular flow regimes differ. For example it is intended not to select any new sites which have clusters similar to these shown in Figure 3.

Results of the cluster analysis indicated little relationship between water quality changes and seasonality. However, a strong relationship exists between these changes and flow regime. Consequently there is little point in collecting samples at regular intervals, but sampling must be done during the different stages of floods.

A three tier system has been proposed (Poplawski and McNeil, 1988), which involves the following components:

(1) A fully automated grid of stations will monitor a limited number of water quality parameters - pH, DO, conductivity and temperature for example. It is expected that some of them will be linked

directly with the'Commission's main office to signal unusual readings.

(2) A limited number of stations will be selected at which samples will be collected manually at prescribed times (after storm events) and an analysis carried out which will include more water quality indicators, mainly nutrients, pesticides and major ions.

(3) Very detailed benchmark surveys in areas of concern will be carried out on an infrequent basis, say every 5 to 10 years. The benchmark surveys will be conducted over a period of about a year. The main purpose of these surveys will be to test correlations between frequently sampled parameters and those sampled only during the benchmark surveys.

Cluster analysis can give a very good indication of the characteristics of groundwater types (McNeil, 1981). The results superimposed on a geological maps clearly indicate the boundary of different water regions. Therefore selection of representative sites becomes an easy exercise, subsequently leading to a reduced number of sampled bores.

As changes in groundwater quality are much slower than in streams, manual sampling at prescribed intervals is proposed. A prototype of a field sampling kit for groundwater is being developed and will be tested in the near future.

Case Study - the Upper Condamine River Catchment

The Upper Condamine Valley (Figure 1), an important agricultural area in south east Queensland, was selected for a pilot study with the aim of establishing a cost effective and efficient water quality monitoring network throughout the state. Its very rich black soil is suitable for growing cotton, sorghum, wheat, barley and corn. Unfortunately, in the past, inadequate land management practices in several areas have resulted in serious land degradation including:

depletion of groundwater resources;

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extensive soil erosion resulting from land clearing, and

deterioration of water quality due to improper farm practices.

The study employed the statistical analyses outlined above to provide a description of the water quality in the area. This was compared with geological maps and satellite images depicting land use, and zones with similar characteristics and needs were mapped out.

Two to three hundred groundwater sites in the Upper Condamine River catchment have been sampled at infrequent intervals over some years, usually when a major water resource assessment was being carried out in a particular locality. Some forty surface water sites have been sampled since the '70s. Because of rising costs, these are expected to be reduced to about eight ground water and five surface water sites, on the assumption that another major survey can take place in five to ten years in order to check correlations, and that conductivities will be monitored on field staff's regular water level and gauging rounds. This is particularly necessary in an area such as Queensland, which is not fully developed, and therefore prone to major landuse changes within less than a decade.

The following diagram illustrates the sequence of procedures which the Commission plans to implement on the Upper Condamine and subsequently on all of the other basins in the state.

CONCLUSION

The procedure described above should lead to a more efficient water quality network without compromising the quality and relevance of data collected. This information will be used for better assessment and management of water resources in Queensland.

ACKNOWLEDGEMENTS

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┌─────────────────────────────────────────────────────────────┐
│             Initial investigation of a basin.                │
└─────────────────────────────────────────────────────────────┘

┌──────────────────┐  ┌──────────────────┐  ┌─────────────────────────────┐
│Study existing data│  │ Collect new data │  │Environmental study of the basin│
└──────────────────┘  └──────────────────┘  └─────────────────────────────┘

┌─────────────────────────────────────────────────────────────┐
│Interpret basic natural water chemistry and main environmental influences.│
└─────────────────────────────────────────────────────────────┘

┌─────────────────────────────────────────────────────────────┐
│Divide basin into subareas with permanent monitoring site(s) and auxiliary│
│   sites (groundwater level and stream gauging sites) within the subarea.  │
└─────────────────────────────────────────────────────────────┘
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Regular sampling of
permanent sites for
limited set of species.

Continuing work on
correlating permanent
and auxiliary sites.

Conductivity taken at
every auxiliary site
maintenance visit ...

... leading to ...

continuous logging of
conductivity at all
water level and
gauging sites.

Publish summaries and maps of water quality for potential
users and managers, and monitor threats to the resource.

Complete re-assessment of network within 5 to 10 years

86

Statistical Aspects of
Monitoring System Design

USE OF BOX PLOTS AND TREND ANALYSES TO EVALUATE SAMPLING FREQUENCY AT WATER-QUALITY MONITORING SITES

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ABSTRACT

Water samples from monitoring sites commonly are collected for chemical analysis at regular time intervals. Determination of the most efficient sampling frequency that does not result in loss of information may be difficult. Box plots of data can provide a convenient visual comparison between the distributions of data for the existing sampling frequency and various decreased frequencies. In this report, box plots are described, and their use in evaluation of sampling frequency is demonstrated by using examples from U.S. Geological Survey water-quality monitoring sites in the South Platte River basin of Colorado. The distributions of data collected at monthly intervals are compared to distributions of subsets of the data selected at bimonthly and quarterly intervals. Results of this evaluation are tested by comparing the significance level of trends identified for the complete data set with those identified using data for the decreased sampling frequencies. The non-parametric seasonal Kendall test is used for trend analyses to avoid potential problems caused by nonnormality, seasonality, and serial dependence in the data sets.

INTRODUCTION

Water samples from monitoring sites commonly are collected for chemical analysis at regular time intervals. Samples must be collected often enough to represent the variations in water quality at the site, but sampling too frequently is unnecessarily expensive. Determination of the most efficient sampling frequency that does not result in loss of information may be difficult. This report describes two methods that can be used to evaluate the potential loss of information that may result if sampling frequency is decreased from monthly to bimonthly or quarterly.

Loss of information caused by decreasing the sampling frequency can be evaluated by the ability of the resultant data set to preserve properties of data that were collected at the original sampling frequency. If a data set from bimonthly sampling has properties similar to those of a data set from monthly sampling, the information lost by decreasing the sampling frequency may be negligible. Two possible criteria for comparing data sets from different sampling frequencies are detectability of trends and similarity of data distributions. The detectability of trends can be compared by testing the significance of monotonic trends, using a method appropriate to the characteristics of the data sets. Data distributions can be compared by testing the equivalence of certain statistics, such as the mean, median, or standard deviation; however, the number of statistics that can be tested is limited, and the tests become complex if more than two data sets are involved. A summary of many distribution properties can be compared by using visual displays, such as the box plot (Tukey, 1977). Similar box plots are an indication of similar data distributions.

DESCRIPTION OF BOX PLOTS

Box plots were proposed by Tukey (1977) to summarize the properties of a data distribution. The median, upper and lower quartiles, and range of the data are shown explicitly in box plots (fig. 1). The box boundaries enclose the central 50 percent of the data, which is referred to as the inter-quartile range (IQR). The vertical lines extend from the quartiles to the largest and smallest data values that are within 1.5 times the IQR. Data values outside this range are plotted individually as outliers. Box plots displayed next to each other can provide an effective visual comparison of many properties for a number of data sets (Chambers and others, 1983).

METHOD OF TREND ANALYSIS

Trend analyses of time-series data for water-quality properties and constituents are complicated by several common character-istics of these data sets: nonnormality, seasonality, serial dependence, and censored values (reported as less than a detection limit). The seasonal Kendall test is a technique unaffected by these characteristics (Hirsch and others, 1982; Hirsch and Slack, 1984). This technique is used to identify significant monotonic changes in the data set over time. The seasonal Kendall test is nonparametric; the test statistic is determined by using ranks of the data, rather than actual data values. Censoring and nonnormality do not affect rank. Trends are evaluated separately for each season (specified as a fraction of the year), and results are combined into a single test statistic (tau). The significance level (p-value) of the test statistic then is adjusted to account for serial correlation.

EVALUATION OF SAMPLING FREQUENCY

The utility of box-plot comparisons and trend analyses in evaluating sampling frequency was tested at three water-quality monitoring sites operated by the U.S. Geological Survey in the South Platte River basin, Colorado (fig. 2). Site 1 is located at the east portal of the Adams Tunnel (Alva B. Adams Tunnel at east portal near Estes Park, station 09013000), which conveys water diverted from the Colorado River basin into the South Platte River basin. Although streamflow at this site is controlled by pumping into the tunnel, the water chemistry is representative of headwater streams in the Front Range of northern Colorado (Liebermann and others, 1988). Site 2 is on Boulder Creek (Boulder Creek at mouth near Longmont, station 06730500) near its confluence with St. Vrain Creek. Water quality at this site is affected by transbasin imports, municipal effluent from the city of Boulder, and a small area of irrigated agriculture in the basin. Site 3 is on the South Platte River (South Platte River near Weldona, station 06758500) downstream from an extensive area of irrigated farmland. Water quality at this site is affected by irrigation diversions and return flows.

All data used in this study were retrieved from the U.S. Geological Survey data base. The retrieval procedure selected all data available for each of the three sites included in the study. The data were reviewed and summarized in a report by D.K. Mueller (U.S. Geological Survey, written commun., 1989). The data sets for each site included on-site measurements of specific conductance, pH, temperature, and dissolved oxygen, and laboratory analyses of major ionic species, nutrients, and trace metals. In addition, bacteria data were available for sites 1 and 2 (Adams Tunnel and Boulder Creek). The period of record retrieved for each site is listed in table 1.

Results of Box-Plot Comparisons

Sampling frequency was approximately monthly during the period of record at each site. The data sets were analyzed to determine whether sampling frequency could be decreased to bimonthly or quarterly without substantial loss of information. Two subsets were used to test bimonthly sampling: (1) Data collected in odd-numbered months (January equals 1), and (2) data collected in even-numbered months. Three subsets were used to test quarterly sampling: (1) Data collected in January, April, July, and October;

○   Far Out Value (> 3 times IQR)

×   Outside Value (> 1.5 times IQR)

Largest Value less than
1.5 times IQR

75th Percentile (Upper Quartile)

Median

25th Percentile (Lower Quartile)

Smallest Value less than
1.5 times IQR
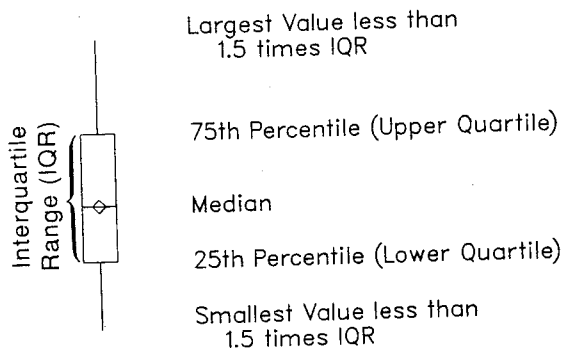
Figure 1. Example diagram of box plot.
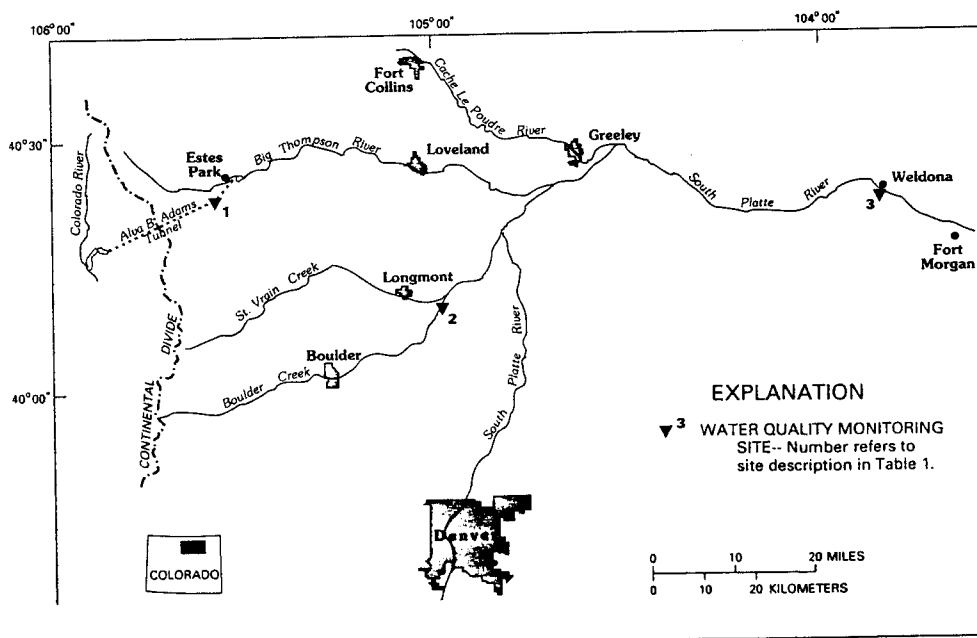
Location of water-quality monitoring sites.

Table 1.--Water-quality monitoring sites

Site number (figure 2)	Station number	U.S. Geological Survey station name	Number of samples	Period of record
1	09013000	Alva B. Adams Tunnel at east portal, near Estes Park	181	1970-87
2	06730500	Boulder Creek at mouth near Longmont	95	1979-87
3	06758500	South Platte River near Weldona	203	1971-87

(2) data collected in February, May, August, and November; and (3) data collected in March, June, September, and December.

For each site, box plots were constructed for each water-quality property and constituent that had sufficient data. The criteria for sufficient data were defined to be: (1) At least 10 values equal to or exceeding the detection limit; and (2) no more than 75 percent of the values less than the detection limit. Because the data for many constituents included censored (less-than) values, medians and quartiles were computed by using estimates of the distribution of data less than detection limits. Gilliom and Helsel (1986) determined that a log-normal maximum-likelihood method was best for estimating the median and quartiles from data sets containing censored values. Helsel and Cohn (1988) modified this method to accept data sets that have more than one detection limit. This modified method was used to compute all medians and quartiles necessary for constructing box plots in this study.

Box plots of selected constituent data from site 1 (Adams Tunnel) are shown in figure 3. For each constituent, side-by-side box plots are displayed for the monthly sampling frequency, for the two possible bimonthly frequencies, and for the three possible quarterly frequencies. By visual comparison, most of the bimonthly data distributions seem to be similar to the monthly data distribution. Only total phosphorus and copper had bimonthly distributions that were substantially different from the monthly distribution and then only for data from the first subset (odd-numbered months). The loss of information caused by decreasing the sampling frequency to bimonthly may be small, particularly if samples are collected in even-numbered months. Comparison of the quarterly and monthly box plots indicates that at least one of the quarterly data distributions is different from the monthly data distribution for four constituents (dissolved solids, total phosphorus, copper, and nickel). This difference indicates that the loss of information caused by decreasing the sampling frequency to quarterly may be substantial.

Box plots for selected properties and constituents from site 2 (Boulder Creek) indicate minimal difference among any of the distributions (fig. 4). Based on this visual inspection, sampling frequency might be decreased to either bimonthly or quarterly without substantial loss of information. Maximum ranges seem more likely to occur in samples from the second bimonthly schedule (even-numbered months) and the first quarterly schedule (January, April, July, and October). Sampling on either of these schedules might preserve not only the distribution but also the minimum and maximum values for many properties and constituents.

Box plots of selected data from site 3 (South Platte River) also are similar for all data subsets (fig. 5). Maximum values occur more often in the first bimonthly data subset (odd-numbered months), but there is no consistent pattern among the quarterly data subsets. Sampling frequency might be decreased to quarterly with little loss of information.

Results of Trend Analyses

Results of the box-plot analyses were corroborated by comparing trends identified in the monthly data set with trends in the bimonthly and quarterly data subsets. If significant trends in the monthly data were not significant in a particular data subset, decreasing the sampling frequency could result in a loss of information. The significance of trends was determined by using the seasonal Kendall test, adjusted for serial correlation. Significant trends were identified based on the following criteria for the significance level (p-value) of the seasonal Kendall test statistic (tau):

Moderately significant -- significance level less than or equal to 0.1 and greater than 0.05.

Significant -- significance level less than or equal to 0.05 and greater than 0.01.

Very significant -- significance level less than or equal to 0.01.

MANGANESE, IN MICROGRAMS PER LITER

TOTAL PHOSPHORUS, IN MILLIGRAMS PER LITER

DISSOLVED SOLIDS, IN MILLIGRAMS PER LITER

NICKEL, IN MICROGRAMS PER LITER

COPPER, IN MICROGRAMS PER LITER

NITRITE + NITRATE AS N, IN MILLIGRAMS PER LITER
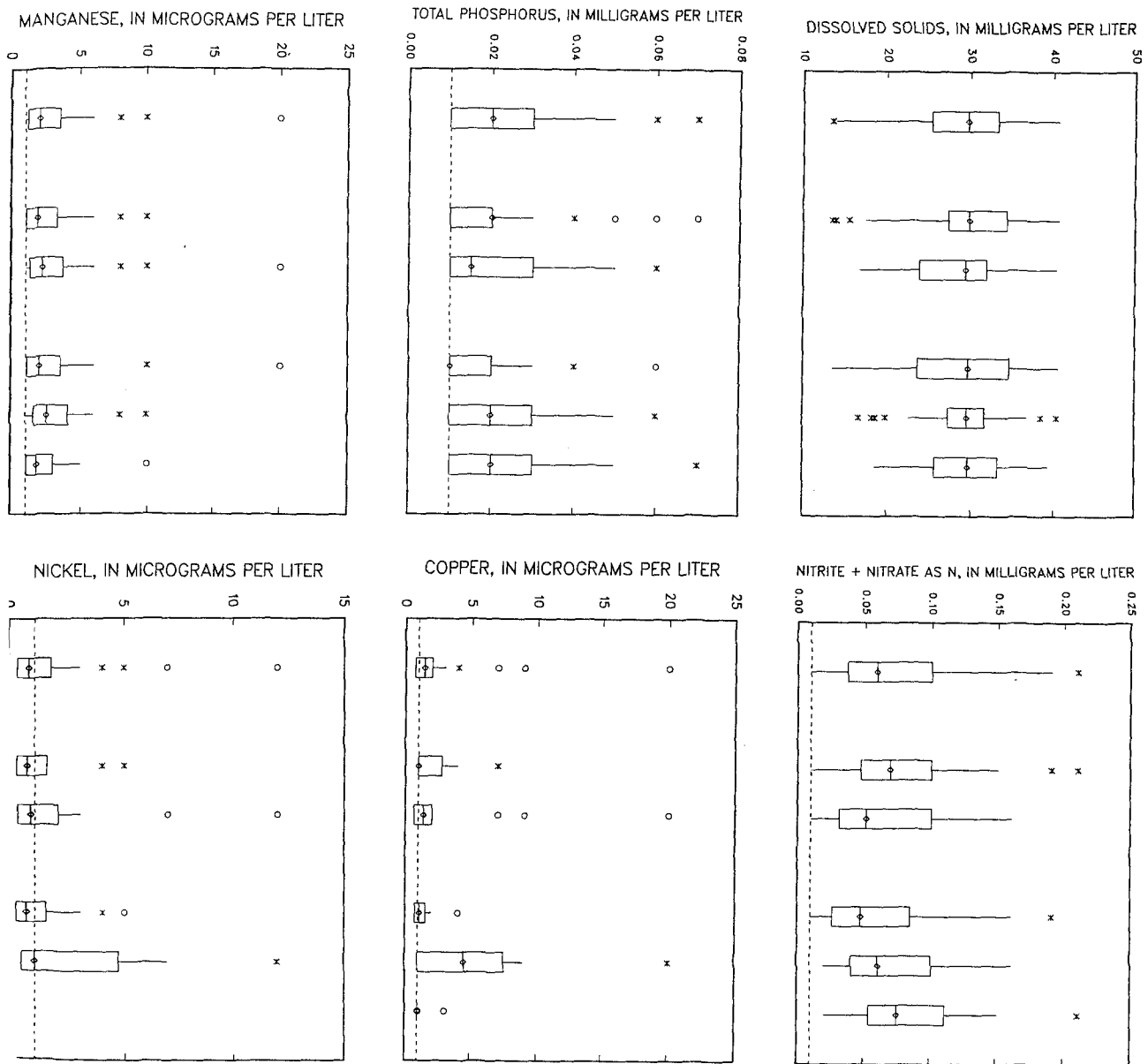
Figure 3.--Box plots of selected data for various sampling frequencies at site 1, Alva B. Adams Tunnel at east portal (dashed line indicates detection limit).

Figure 4.--Box plots of selected data for various sampling frequencies at site 2, Boulder Creek at mouth near Longmont.
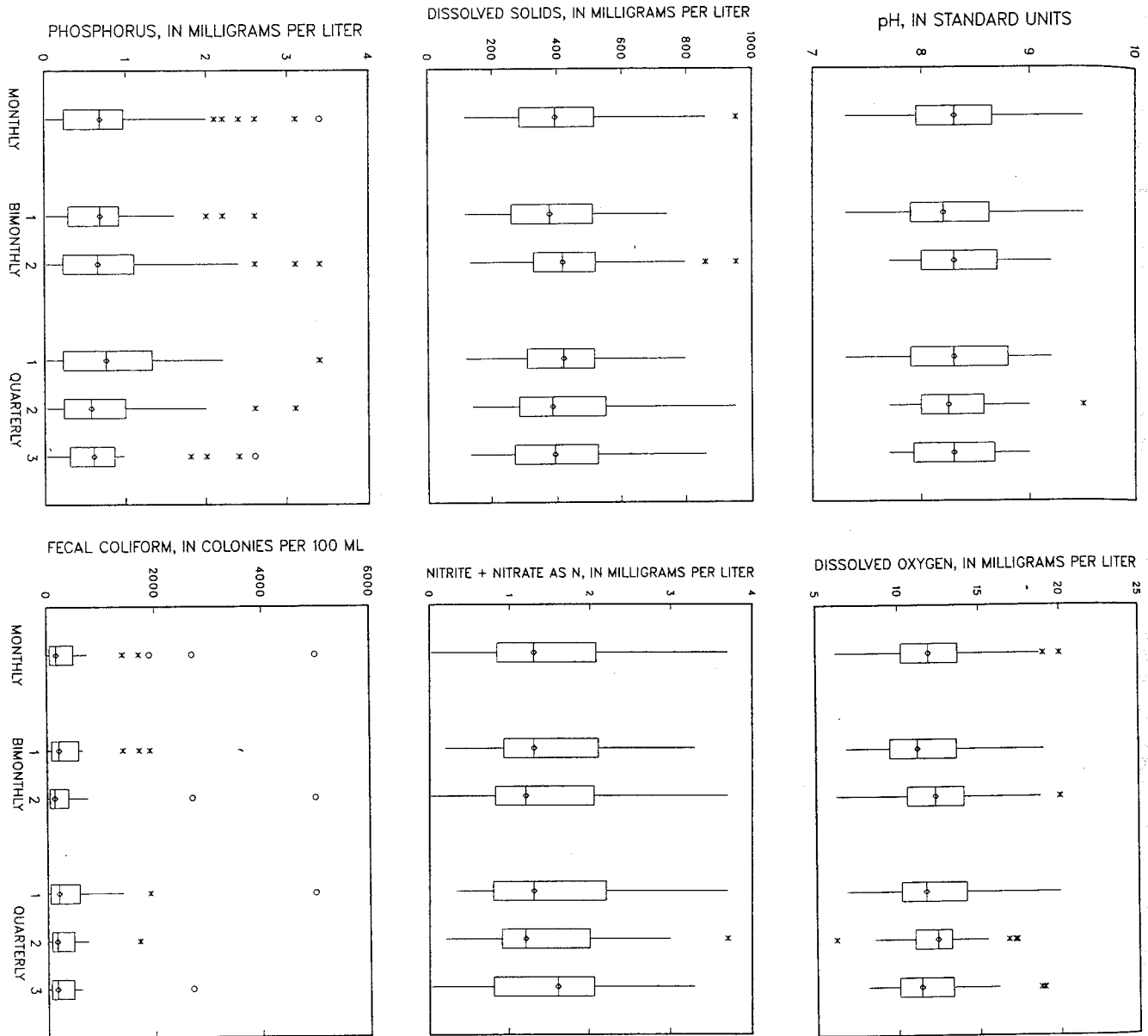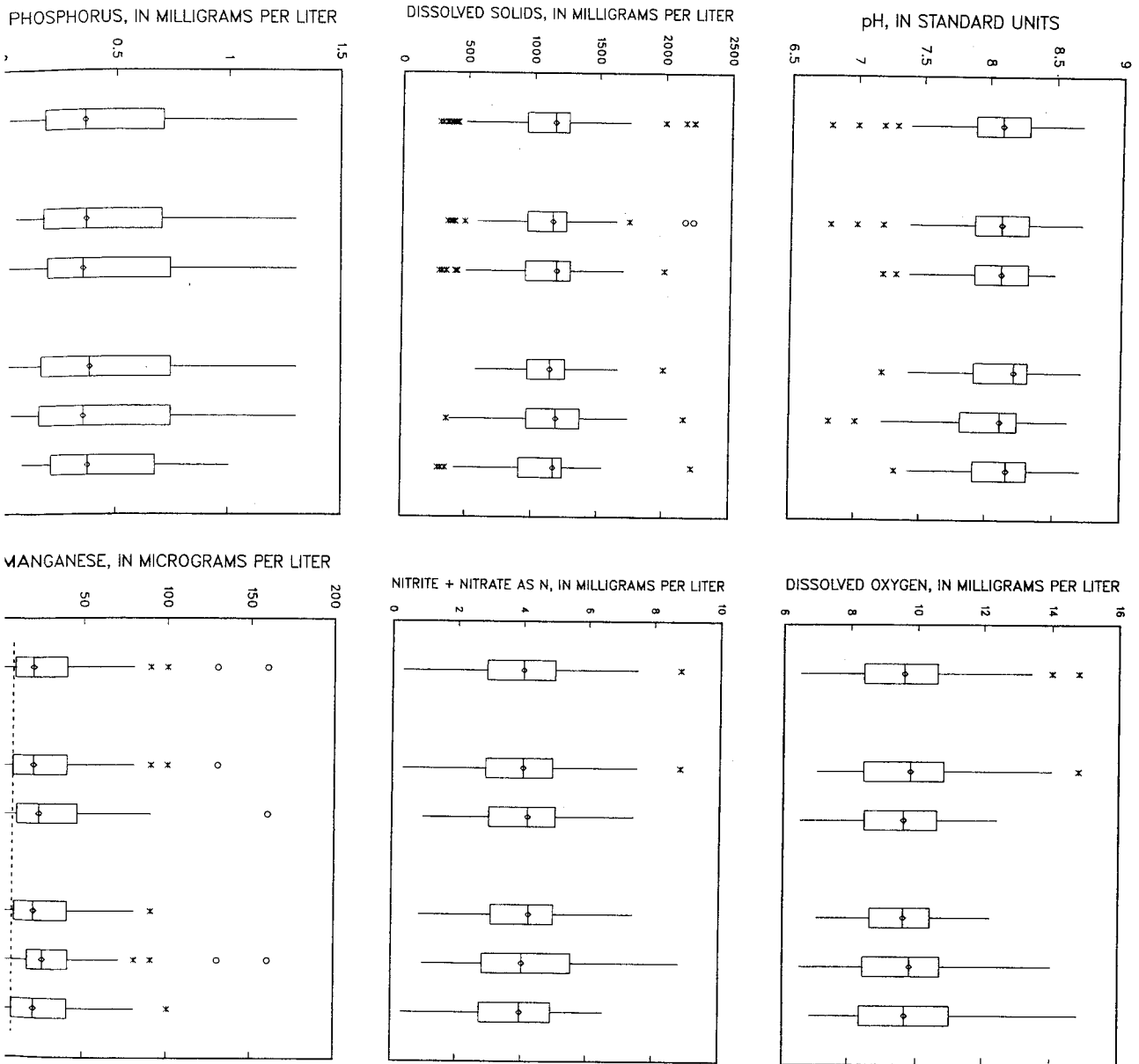
Figure 5.-- Box plots of selected data for various sampling frequencies at site 3, South Platte River near Weldona (dashed line indicates detection limit).

In addition to testing the original data, the seasonal Kendall test also was used to identify trends in the time series of flow-adjusted concentrations. Flow adjustment is used to eliminate the effect of correlation between streamflow and water-quality property or constituent values (Hirsch and others, 1982). This adjustment decreases the possibility of misinterpreting the significance of a trend in water quality that results only from a change in streamflow during the period of record. In this study, flow-adjusted concentration was defined to be the residual (actual minus estimated value) from linear regression of each property or constituent on the logarithm of streamflow. (Actual pH was used, because it is already a logarithm.) Flow adjustment procedures were not used in trend analysis of data from site 1 (Adams Tunnel), because the flow was completely controlled by pumping, and no correlation with water quality was expected.

The significance levels of trends for various sampling frequencies for data from site 1 (Adams Tunnel) are summarized in table 2. Five trends were identified in the monthly data. At least four of these trends still could be identified in either bimonthly data subset. However, in one of the quarterly data subsets (Quarterly 1), only two of the trends still could be identified. These results confirm the implication from the box plot comparisons that the loss of information caused by decreasing the sampling frequency might be small for bimonthly sampling but could be substantial for quarterly sampling.

Some idea of the information loss is provided by the decrease in significance of trends that occurs as the sample size is decreased. At site 1 (table 2), the significance of the trend in specific conductance is the same for monthly and bimonthly data, but it is less significant for each quarterly data subset. The trend in calcium is less significant for both bimonthly data subsets than for the monthly data, but retains most of its significance in the Quarterly 2 data subset that includes February, May, August, and November. Data from these months seem to produce much of the trend identified in the monthly data set. These results provide

additional information about when sampling should be scheduled if the frequency is decreased.

The significance of trends for data from site 2 (Boulder Creek) are summarized in table 3. Five trends were identified in the monthly data for a variety of properties and constituents: temperature, sulfate, nitrite plus nitrate, iron, and fecal-coliform bacteria. Three or four of these trends still could be identified in the bimonthly data subsets, but only two trends still could be identified in two of the quarterly data subsets. In addition, a trend in phosphorus that did not exist in the monthly data was identified in one quarterly subset. These results contradict those of the box-plot comparisons. The trend analyses indicate that loss of information may be substantial if sampling frequency is decreased to quarterly. However, the trend analyses and box-plot comparisons indicate that bimonthly sampling would cause only a small loss of information.

Sixteen trends were identified in the monthly data from site 3 (South Platte River, table 4). Eleven of these trends were associated with major ionic species or related properties, such as specific conductance, hardness, and dissolved solids. These eleven trends were very significant, even for flow-adjusted data. Trends also were identified for pH, nutrients, and manganese. At least 15 trends still could be identified in the bimonthly data subsets, and at least 13 trends could be identified in each of the quarterly data subsets. All 16 of the monthly trends were identified in data from the Quarterly 3 subset. Minimal information may be lost if the sampling frequency were decreased to quarterly at this site, particularly if samples were collected during the months comprising the Quarterly 3 data subset (March, June, September, and December). A trend in chloride that did not exist in the monthly data was identified in the Quarterly 3 subset, but it was less significant than the trends in other major ionic species and, therefore, does not indicate much loss of information. Results of the trend analysis confirm the box-plot comparisons and additionally provide a basis for scheduling sample collection.

Table 2.--Significance of trends for various sampling frequencies at site 1,

Alva B. Adams Tunnel at east portal near Estes Park

[o, insignificant trend or no trend; *, moderately significant trend;

, significant trend; *, very significant trend]

Property or constituent[1]	Significance of trend for indicated sampling frequency[2]					
	Monthly	Bimonthly 1	Bimonthly 2	Quarterly 1	Quarterly 2	Quarterly 3
Specific conductance	***	***	***	**	**	**
pH	o	o	o	o	o	o
Temperature	o	o	o	o	o	o
Dissolved oxygen	o	o	o	o	o	o
Hardness (as $CaCO_3$)	**	**	*	o	**	*
Dissolved solids	o	o	o	o	o	o
Calcium	**	*	*	o	**	*
Magnesium	**	**	o	*	o	o
Sodium	**	*	*	o	*	*
Potassium	o	o	o	o	o	o
Alkalinity (as $CaCO^3$)	o	o	o	o	o	o

Table 2.--Significance of trends for various sampling frequencies at site 1, Alva B. Adams Tunnel at east portal near Estes Park--Continued

Property or constituent[1]	Significance of trend for indicated sampling frequency[2]					
	Monthly	Bimonthly 1	Bimonthly 2	Quarterly 1	Quarterly 2	Quarterly 3
Chloride	o	o	o	o	o	o
Sulfate	o	o	o	o	o	o
Fluoride	o	o	o	o	o	o
Silica	o	o	o	o	o	o
Ammonia + organic N, total	o	o	o	o	o	o
Iron	o	o	o	o	o	o

[1]Constituent concentration is dissolved unless otherwise indicated.

[2]Bimonthly 1 = Samples from odd numbered months (January = 1);

Bimonthly 2 = Samples from even numbered months;

Quarterly 1 = Samples from January, April, July, and October;

Quarterly 2 = Samples from February, May, August, and November;

Quarterly 3 = Samples from March, June, September, and December.

Table 3.--Significance of trends for various sampling frequencies

at site 2, Boulder Creek at mouth

[o, insignificant trend or no trend; *, moderately significant trend; **,

significant trend; ***, very significant trend; parentheses indicate

flow-adjusted data]

Property or constituent[1]	Significance of trend for indicated sampling frequency[2]					
	Monthly	Bimonthly 1	Bimonthly 2	Quarterly 1	Quarterly 2	Quarterly 3
Specific conductance	(o)	(o)	(o)	(o)	(o)	(o)
pH	o	o	o	o	o	o
Temperature	***	*	**	*	*	o
Dissolved oxygen	o	o	o	o	o	o
Hardness (as $CaCO_3$)	(o)	(o)	(o)	(o)	(o)	(o)
Dissolved solids	(o)	(o)	(o)	(o)	(o)	(o)
Calcium	(o)	(o)	(o)	(o)	(o)	(o)
Magnesium	(o)	(o)	(o)	(o)	(o)	(o)
Sodium	(o)	(o)	(o)	(o)	(o)	(o)
Potassium	o	o	o	o	o	o
Alkalinity (as $CaCO_3$)	(o)	o	(o)	(o)	(o)	(o)
Chloride	o	o	o	o	o	o
Sulfate	(**)	(*)	(o)	(o)	(o)	(o)
Fluoride	o	o	o	o	o	o

Table 3.--Significance of trends for various sampling frequencies

at site 2, Boulder Creek at mouth--Continued

Property or constituent[1]	Significance of trend for indicated sampling frequency[2]					
	Monthly	Bimonthly 1	Bimonthly 2	Quarterly 1	Quarterly 2	Quarterly 3
Silica	o	o	o	o	o	o
Nitrite + nitrate (as N)	***	*	**	o	*	**
Phosphorus	o	o	o	o	o	*
Iron	***	***	***	***	*	**
Manganese	o	o	o	o	o	o
Fecal coliform	**	o	o	o	o	o
Fecal streptococcus	o	o	o	o	o	o

[1]Constituent concentration is dissolved unless otherwise indicated.

[2]Bimonthly 1 = Samples from odd numbered months (January = 1);

Bimonthly 2 = Samples from even numbered months;

Quarterly 1 = Samples from January, April, July, and October;

Quarterly 2 = Samples from February, May, August, and November;

Quarterly 3 = Samples from March, June, September, and December.

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Table 4.--Significance of trends for various sampling frequencies

at site 3, South Platte River near Weldona

[o, insignificant trend or no trend; *, moderately significant trend; **,

significant trend; ***, very significant trend; parentheses indicate

flow-adjusted data]

Property or constituent[1]	Significance of trend for indicated sampling frequency[2]					
	Monthly	Bimonthly 1	Bimonthly 2	Quar-terly 1	Quar-terly 2	Quar-terly 3
Specific conductance	(***)	(***)	(***)	(**)	(***)	**
pH	**	**	**	**	o	**
Temperature	o	*	o	*	o	o
Dissolved oxygen	o	o	o	o	o	o
Hardness (as CaCO₃)	(***)	(***)	(***)	(**)	(***)	(***)
Dissolved solids	(***)	(***)	(***)	(**)	(***)	(***)
Calcium	(***)	(***)	(***)	(**)	(***)	(***)
Magnesium	(***)	(***)	***)	(**)	(***)	(***)
Sodium	(***)	(***)	(***)	(*)	(***)	(**)
Potassium	(***)	(***)	**	(*)	(***)	(**)
Alkalinity (as CaCO₃)	***	***	***	***	***	**

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Table 4.--Significance of trends for various sampling frequencies
at site 3, South Platte River near Weldona--Continued

Property or constituent[1]	Significance of trend for indicated sampling frequency[2]					
	Monthly	Bimonthly 1	Bimonthly 2	Quarterly 1	Quarterly 2	Quarterly 3
Chloride	o	o	o	o	*	*
Sulfate	(***)	(***)	(***)	(**)	(***)	(***)
Fluoride	***	**	***	***	*	**
Silica	***	***	***	***	***	***
Nitrite + nitrate (as N)	**	**	o	o	o	*
Orthophosphate (as P)	***	**	***	***	***	**
Phosphorus	***	**	***	o	*	**
Manganese	***	**	***	o	*	**

[1]Constituent concentration is dissolved unless otherwise indicated.

[2]Bimonthly 1 = Samples from odd numbered months (January = 1);

Bimonthly 2 = Samples from even numbered months;

Quarterly 1 = Samples from January, April, July, and October;

Quarterly 2 = Samples from February, May, August, and November;

Quarterly 3 = Samples from March, June, September, and December.

Interpretation of results

For each of the selected sites, comparisons of box plots of the data distributions and of trend analyses indicate that monthly sampling may not be necessary to describe the quality of water in a long-term monitoring program. Although these results may not be conclusive, they provide an indication as to what sampling frequency might be appropriate and which property or constituent data might be affected by a decrease in sampling frequency. Additional tests are needed to confirm that the loss of information is small. Such tests could include comparison of the variance in estimating the mean annual concentrations, based on the covariance among samples. If monthly values are highly correlated, the variance in mean annual concentration may not be affected by a decrease to less frequent sampling. Also, comparison of monthly box plots could be used to evaluate seasonality in the data and to provide more information about when samples need to be collected. The two methods used in this study are easily performed and could be used as screening procedures to indicate sites where a decrease in sampling frequency should be more thoroughly investigated.

SUMMARY AND CONCLUSIONS

Analysis of sampling frequency at streamflow sites was based on comparisons between the entire data set and selected subsets. Data subsets were selected to represent decreased sampling frequencies at bimonthly or quarterly intervals. Comparisons were made of distributions of water-quality data using box plots and trend analysis. Based on visual inspection of box plots, a small loss of information might be expected if the sampling frequency is decreased to bimonthly at one site (Adams Tunnel at east portal) and to quarterly at two sites (Boulder Creek at mouth and South Platte River near Weldona). Comparison of trends identified by using the seasonal Kendall test supported these conclusions for the Adams Tunnel and South Platte River sites but indicated that a substantial loss of information might occur if

sampling at the Boulder Creek site is decreased to less than bimonthly. Based on the overall analysis, data collected bimonthly at the Adams Tunnel and Boulder Creek sites and quarterly at the South Platte River site might provide essentially the same information as does data collected monthly.

The box-plot comparison and trend-analysis techniques provide a convenient and useful method for examining the efficiency of sampling frequency at water-quality monitoring sites. Application of both techniques is necessary for corroboration of evidence that decreasing the sampling frequency could result in minimal loss of information. If sampling frequency can be decreased, the box plots and trend-analysis results also provide a basis for selecting a sampling schedule.

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AN INFORMATION SYSTEM FOR AGRICULTURAL CHEMICALS IN RURAL, PRIVATE, WATER-SUPPLY WELLS

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BACKGROUND

The Illinois State Geological Survey (ISGS) and the Illinois State Water Survey (ISWS), divisions of the Illinois Department of Energy and Natural Resources (IDENR) have developed a design for a statewide survey of rural private wells to assess the occurrence of agricultural chemicals (pesticides and nitrates) in them (McKenna, et al., 1989). The project is the first agricultural-chemical related response to the mandates of the Illinois Groundwater Protection Act (IGPA) of 1987. One mandate of the act was that IDENR evaluate the impact of agricultural chemicals on ground- water, particularly in rural areas where pesticides are used most intensively. Also included in the IGPA is a mandate to IDENR to develop a database related to groundwater information for the State. These 2 mandates were the driving forces behind the design of the Illinois study and information system.

In Illinois, the concern over the potential for agricultural chemical contamination of groundwater is based on these facts:

Agricultural chemicals are extensively used.

Groundwater is the source of drinking water in many rural areas.

Aquifers occur at shallow depths throughout the state.

Pesticide contamination of ground-water water has been found in other mid-western states with climate, soils, geology, and agricultural practices similar to Illinois.

Knowledge of the extent of agricultural chemical contamination of groundwater in Illinois remains limited. Previous sampling programs by the Illinois Environmental Protection Agency (IEPA), the Illinois Department of Public Health (IDPH), and the ISGS have analyzed for relatively few compounds and only sampled public water-supply wells or wells thought to be highly vulnerable to contamination. Statewide groundwater monitoring plans have been developed over the past 5 years (O'Hearn and Schock, 1985; Shafer et al., 1985), and components of each have been incorporated into sampling programs conducted by the IEPA. However, none of these monitoring plans was designed to assess the occurrence of agricultural chemicals in groundwater. A national pesticide survey (NPS), currently being conducted by the United States Environmental Protection Agency (USEPA), will also sample wells in Illinois; but data appropriate for describing conditions at the state level will not be generated (Mason et al., 1987).

STUDY DESIGN

The study design maximizes the acquisition of data on the potential exposure of the rural population of Illinois to agricultural chemicals through their drinking water. Sampling existing wells minimizes network establishment costs and reflects the water being consumed by the rural population.

The key elements of the experimental design are:

* sample population - drilled, rural, private water-supply wells;

* analytes chosen based on use in Illinois and potential to contaminate ground-water;

* stratified random sampling design using the potential for contamination of shallow aquifers as the stratification variable;

* random selection of wells within each strata;

* characterization of well sites and identification of potential sources of contamination;

* sampling schedule that addresses temporal variability;

* detailed protocols for all phases of the study;

* use of USEPA NPS analytical methods;

* rigorous quality assurance/quality control procedures;

* development of an integrated agricultural-chemical information system.

* recommendations for project organization and management;

* guidelines for data management, statistical analysis, and interpretation of survey results.

AUTOMATED AGRICULTURAL-CHEMICAL INFORMATION SYSTEM

The information derived in this effort will be stored in a PC-based, integrated relational database management system. The software for system will be based on the R-Base for DOS relational database management package. The final product will include information gathered and developed in all phases of the agricultural-chemical study. Well-specific information for each well in the system will be maintained. The system will serve the staff throughout all phases of the study. It will

help in planning of sampling schedules, tracking samples from collection to the reporting of the results, keeping laboratory efforts in control, interpretation of results, and generating output reports of several kinds. It is important that the system be accessible to the field staff through the use of portable, lap-top computers to be used during the well-site observation, the interviews with the well owner/users, and for recording field measurements. The system must be available to the laboratory staff to log in samples, record results, note problems and questions, and track quality assurance/ quality control information. Project staff will have access to the entire system in order to check schedules, and keep materials available, to interpret results, and to produce reports.

SOURCES OF INFORMATION IN THE SYSTEM

There are 5 phases of effort in the study from which information will be taken. The phases are:

I. Planning
II. Verification
III. Field Work
IV. Laboratory Work
V. Reporting

Phase I - Planning

During the planning phase of the study, a Geographic Information System (GIS) was used extensively to combine data from existing studies and previous research. These data included depth to aquifer, pesticide use in Illinois based on corn and soybean cropping patterns, and urban/non-urban status of land surface. The information was combined to produce a map of the potential for contamination by agricultural chemicals (Figure 1). The attribute data from these mapping exercises will be stored in the information system for future reference and mapping.

Equally important in the planning phase of the study is the contacting of county officials to compile more detailed information than is available for private, rural wells in the

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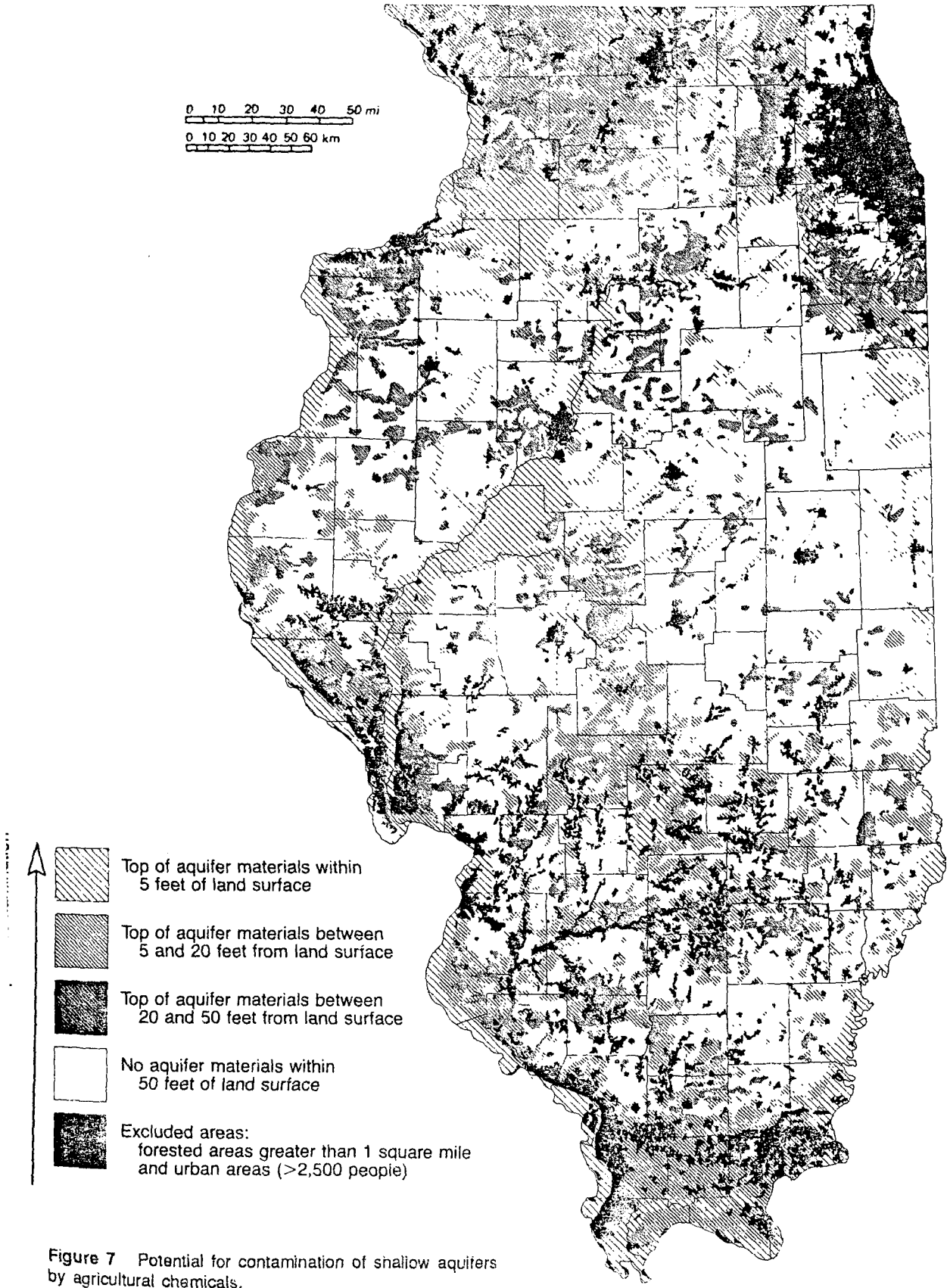
Figure 7 Potential for contamination of shallow aquifers by agricultural chemicals.

Legend:

- Top of aquifer materials within 5 feet of land surface
- Top of aquifer materials between 5 and 20 feet from land surface
- Top of aquifer materials between 20 and 50 feet from land surface
- No aquifer materials within 50 feet of land surface
- Excluded areas: forested areas greater than 1 square mile and urban areas (>2,500 people)

Figure 1. Potential for Contamination by Agricultural Chemicals

existing paper files. The data from those contacts include location of farms and wells, farm-specific agricultural practices, the name of the current owner/ user of the wells, and any available information about recent accidents related to agricultural chemicals.

Phase II - Verification

As part of a cross-referencing and verification of private well data, existing files at both the ISWS and the ISGS will be reviewed. The review will establish what is known about the private rural wells. Local subsurface geology from well logs, well age, construction details, and well history will be tabulated for each private well selected for sampling.

It will be very important to keep this information for each well in the information system. It will be important during the planning phase to verify that selected wells actually tap the aquifer materials of the strata to which the well has been assigned. The data will be used for reanalysis of chemical analytical results in the later phases of the study.

Phase III - Field Work

After the establishment of the areas for each of the strata, 3 segments of field work will occur. These are a well-site observation, a well owner/user interview, and collection of field measurements of physical and chemical parameters at the time of sample collection.

Well-site Observation

Once the strata within which wells will be selected have been determined, and the wells are specified, a well-site observation will be carried out. A trained staff member will visit the site to obtain detailed information about the physical setting of the well and the area proximal to that well. A form has been developed for this well-site observation. The data collected will include uses of the well, availability of the well for sampling, and materials on the surface at, and near, the

well. All of the information collected during the well-site observation will be kept in the information management system. The well-site observation questionnaire appears in Appendix A.

Well owner/user interview

A well owner/user interview will be performed by trained staff prior to the beginning of the water sample collection phase of the study. Detailed information about the status, uses, construction, and history of the well will be collected during this interview. Questions are targeted to determine general information about the well, agricultural practices, and chemical accidents which could affect the water from that well. A separate section of the interview will deal specifically with pesticide use in the vicinity of the well. In both the general information, and pesticides information sections of the interview, the interviewer will record whether the answers to the questions are given from memory, from observation by the owner/user, or from records. This information is expected to be useful in determining the accuracy and dependability of the collected data. A portion of the Well Owner/User questionnaire appears in Appendix B.

Field Parameter Measurements

At the time of water sample collection, pH, electrical conductivity, and water temperature will be determined and recorded. These data will be entered into the information system along with any comments made by field personnel. This information will be useful in interpretation of results and in determining if there are any extenuating circumstances which might prohibit the inclusion of some information from the final analyses. The chain-of-custody of the water samples will be tracked on a form which has been prepared for this purpose. The chain-of-custody data will be kept in the information system.

Phase IV - Laboratory Work

The results of chemical analyses, quality assurance/quality control data, and all

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comments by laboratory staff will be carried in the information system. The chain-of-custody will continue through the laboratory process. A chemical analysis form has been developed to record the results of the laboratory work.

Phase V - Reporting

Reporting as used here is a general term which includes the transfer of information to project staff for tracking materials, field activities, sample status, and results. It also includes the return of pertinent information to well owner/users, and the cyclic generation of summaries and detailed data resulting from the study.

Procedures for sorting and assembling the information from all the phases of the study will be prepared as part of the system. Formats for reporting results of specific well analyses to the well owner/user will be prepared. Tracking of materials, samples, and results will be facilitated for project staff with prepared forms and output formats. These formats will be developed with the cooperation of the staff who will be using them. Standard formats for results will be developed for reporting on a regular cycle to sponsors, the legislature, the public, and those agencies involved in the study.

WELL-SPECIFIC IDENTIFICATION NUMBER

Each well in the study will be assigned a unique 4-digit identification number. This number will never be assigned to any other well. If a well is deleted from the system for any reason, the number will not be reassigned to any other well, it will seem to disappear from the system, but the number will be carried in a list which tells of the fate of all numbers. The data in the information system will be related in all tables and files based on this primary key, the well identification number. This number will allow the information from the various tables in the database system to be cross-referenced by specific well. The 4-digit well identification number will be associated with all information for that well. In order to facilitate this aspect of the work,

an extended identification number will be created. The extended identification number will be composed of the 4-digit well ID, a 2-digit sample type number, and a 1 character episode indicator. For example:

Well ID Number	Sample Type Number	Episode Indicator
3647	02	A
	(sample for method 3)	(1st time this well was sampled)
3647	13	B
	(sample for QA/QC for 2method 1)	(2nd time this well was sampled)

Secondary keys will allow cross-referencing and subsetting of the chemical analytical results on the basis of well depth, date of collection, near-well environmental factors, or any other of the data elements in the system. After all wells have been sampled, restratification of the results of the chemical analyses from the wells will allow estimates of the significance of the restratification factors to be made. This technique, called double sampling, has a lower level of confidence than stratified random sampling because the distribution of wells across the various strata cannot be controlled in retrospect. That fact was considered in the selection of the initial sample size so that restratification might still yield groups of a large enough size to analyze with a reasonable level of confidence.

PILOT STUDY

The ISGS and ISWS have received funding to conduct the 3-year, pilot study in cooperation with the IDOA to field test and evaluate the protocols and procedures developed in the plan. The pilot study will also allow a small-scale trial of the information system. This will make it possible to determine if the flow of information into, through and out of the system is efficient, clear, and adequate.

SYSTEM REQUIREMENTS

The information management will require an IBM compatible computer with at least 20 megabytes of hard-disk storage. The tasks of each phase of the study may require varied amounts of storage disk. Project management staff involved with all parts of the work may require larger storage media if they wish to maintain all information on-line. Separate system backup is recommended. Tape, bernoulli disk, high density diskette, or other available media could be used. The computer will have to have an 80286 or 80386 CPU, Hercules compatible graphics, EGA, or VGA cards, and a printer. R:Base for DOS software will be needed.

COMPLICATING ISSUES

The direction of development of the system has been influenced by several complicating factors which make it different from a system developed by one person or group for its own use. These complicating factors are:

* multiple agencies will participate in the study, and therefore will use the system;

* the study will continue for several years, and possibly will become a "permanent" activity;

* data will be analyzed and reanalyzed. As it accumulates, more interpretation and analyses will be possible;

* the information system is targeted to be the basis for future studies.

The comprehensive integrated information system will have to serve personnel from multiple agencies. The statewide survey is planned to be an interagency cooperative effort. Each agency has its own philosophy of information management and its own computer system. Therefore, this system should be as user-friendly as possible, so that staff from all agencies can access it and use it with approximately equivalent success. The system should not require in-depth knowledge of the package or computer. It should, however, allow a user with some knowledge of

the package and/or system to make use of the system in a more sophisticated manner, if desired.

The statewide survey will take two years. Recommendations for long term, continued monitoring have been made. This system will include the results of that monitoring for trend analysis and for determining evolving problems. The system will have to handle input for many years. As analysis and reanalysis of information are indicated or desired, the system will have to be flexible enough to allow it.

If the system is maintained, the information in it will form the foundation for future research. It is expected that the software will be updated over time, as new versions of the R:Base package become available. One of the stated goals of the R:Base package is that it be upwardly compatible. This will allow the procedures developed for these first stages of work to be used in the future. Procedures should be updated and made more responsive to evolving in the future. If the structure of the stored information is kept as simple as possible and is documented from the beginning, updating, upgrading, and more sophisticated uses should be relatively simple to achieve.

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Rural Private Water Well Survey for Agricultural Chemicals

Well-Site Observation

WELL IDENTIFICATION NUMBER _____
(Base number for sample)

_____

Staff member _____ Date of survey _____
Owner Name _____ Phone Number _____

　　　Location of Well _____

　　　Legal Description of Well:

　　　　　　　Twn _____ Rng _____ Sec _____

　　　　　　　Ten Acre Plot _____
　　　　　　　　　and/or

　　　　　Quarter-quarter-quarter section _____

Type of well:

　　　Drilled _____　Dug/Bored _____　Sandpoint _____

　　　Well depth: _____　Year drilled/dug _____

NOTE ANY LIMITATIONS ON ACCESS _____

_____

Please answer the following questions as carefully as possible:

1. What is this well used for?

　　　Private Water Supply _____
　　　Animal Water Supply _____
　　　Irrigation　　　　　　_____
　　　Other (Specify)　　　　_____
　　　Is the well used for more than one purpose? If so,
　　　　　what are they?_____

IF THE WELL IS NOT USED FOR PRIVATE WATER SUPPLY, REPORT THIS
INFORMATION TO THE PROJECT MANAGER SO THAT AN ADDITIONAL WELL
CAN BE SELECTED.

2. Can the well be sampled?

　　　No　　　 _____
　　　Yes　　　 _____
　　　Unknown _____

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3. If the well can be sampled, can the sample be collected before
the treatment point?

     No   _____
     Yes   _____
     Unknown   _____

4. Can the sample be collected before the holding tank?
   (if applicable)

     No   _____
     Yes   _____
     Unknown   _____

5. What is the topographic setting of the well? (check one)

   The well is located on/in a

     Hilltop   _____
     Hillside   _____
     Flat Valley   _____
     Depression   _____
     Other (Specify) _____
     Unknown   _____

6. Is the well open or closed at the surface?

     Open   _____
     Closed   _____
     Unknown   _____

7. Is the well protected at the surface?

     No   _____
     Yes   _____
     Unknown   _____

         If yes, how?

              Well house or shed   _____
              Concrete pad   _____
              Sanitary or grouted seal _____
              Covered pit   _____
              Other (Specify)   _____

8. Is this protection adequate to prevent seepage into the well?

     Yes _____   No _____   Unknown _____

9. Are there any of the following within 500 feet of the well?

Body of water   _____
          Type _____
Drainage ditch
Septic Tank   _____
Septic Field   _____
Cesspool   _____
Animal Grazing Area
Animal Housing Facility   _____
Pesticide Mixing Point   _____
Pesticide Storage   _____
Crop Storage   _____
Irrigation Well   _____
Farmland   _____

If in farmland;

In use now?   _____
What kind of crops?   _____
In use in the past? How long ago?   _____

10. If the soil within 500 feet of the well is not exposed, how is it covered?

Roofed or covered   _____
Paved   _____
Graveled   _____
Rock   _____
Grass/Vegetation   _____
Other cover (Specify) _____
Unknown   _____

11. Is the well water treated? (Mechanically or chemically)

No   _____
Yes   _____   Mechanically   _____
               Chemically   _____

How? (Describe the treatment)

_____

12. Describe and show the location of the sampling point.

Please answer the following questions as carefully as possible:

Staff: Please indicate the source of the answers to these
        questions by circling one of the following letters:
        Memory = M   Observation = O   Records = R

GENERAL INFORMATION SECTION:

1. Do you have copies of a log or other documents about this well?

    Yes _____
    No _____
    Unknown _____

2. In what year was the well drilled or constructed?
                                                        M O R
    _____

        Unknown _____

3. Who drilled the well? _____ M O R

4. Were you the user when the well was drilled?

    Yes _____
    No _____

If not, who was the user?

    _____ M O R
    Unknown _____

5. What is the depth of the well? _____   M O R
            Unknown _____

6. What is the static water level for this well?   M O R
        _____ feet
        Unknown _____

    How long does it take for the water level to
    recover in the well once the pump has been turned off?

    _____
    Unknown _____

7. Has the well been deepened since it was drilled?

    Yes _____   M O R
        What was the previous depth? _____
    No _____
    Unknown _____

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8. What is the diameter of the well in inches of:

the hole drilled for the well
outside the casing? _____   M   O   R
            unknown _____

the inside of the well   _____   M   O   R
            unknown _____

9. In what type of material is the well finished?   M   O   R

Limestone/Dolomite   _____

Sandstone   _____

Sand & Gravel   _____

Other Unconsolidated Material_____
          Describe _____

Unknown   _____

10. Does this well have a casing? (i.e. a protective
covering used to line the well hole)

        Yes   _____   M   O   R
        No   _____
           Unknown _____

11. What material was used to case the well?

Plastic Pipe (PVC)   _____   M   O   R

Concrete or cement   _____

Metal   _____

Tile, brick, or stone   _____

Other (Specify)   _____

Unknown   _____

12. Is the well cased to its total depth?

        Yes   _____   M   O   R
        No   _____
        Near Surface Only   _____
        Distance below ground   _____
           Unknown   _____

(There are 4 more pages of questions in this part)

Pesticide Use

This part of the survey is concerned with the usage of pesticides near this well. Pesticides include all insecticides, herbicides, fungicides, nematicides, rodenticides, and other chemical agents except fertilizers.

35. Have any pesticides been used, mixed, stored, or loaded within 500 feet of the well in the past year?

    Yes _____   Used _____ Mixed _____ M O R
         Stored _____ Disposed _____

    How was it stored? (In the open, in
    a shed,...)_____
    No   _____
    Unknown _____

    Has this happened in the past 2 years?

    Yes _____   Used _____ Mixed _____ M O R
         Stored _____ Disposed _____

    How was it stored? (In the open, in
    a shed,...)_____
    No   _____
    Unknown _____

    (etc)
36. Is water from the well used to mix pesticides
    for spraying?   M O R
    Yes _____
         Is water taken directly from the well to the
         sprayer tank? Yes _____
                       No _____
                       Unknown _____
         Has the sprayer tank ever overflowed?
                       Yes _____ When? _____
                       No _____
                       Unknown _____

         Has the tank ever back-siphoned?
                       Yes _____ When? _____
                       No _____
                       Unknown _____

No   _____
Unknown_____

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37. Starting with this year, back through 1986, what pesticides have been used within 500 feet of the well? (give either the brand name or the active ingredient)

1988 _____   M O R

_____
Unknown _____
How close to the well (in feet) _____
Unknown _____

1987 _____   M O R

_____
Unknown _____
How close to the well (in feet) _____
Unknown _____

1986 _____   M O R

_____
Unknown _____
How close to the well (in feet) _____
Unknown _____

38. Starting with this year, back through 1986, what pesticides have been stored within 500 feet of the well? (give either the brand name or the active ingredient)
(etc)

39. Starting with this year, back through 1986, what pesticides containers have been disposed of within 500 feet of the well? (give either the brand name or the active ingredient)
(etc)

40. Starting with this year, back through 1986, what pesticides have been accidentally spilled down or within 500 feet of the well? (give either the brand name or the active ingredient)
(etc)

41. Starting with this year, back through 1986, what pesticides have been accidentally back-siphoned into the well? (give either the brand name or the active ingredient)
(etc)

DETERMINING AND INCREASING THE STATISTICAL SENSITIVITY OF NONPOINT SOURCE CONTROL GRAB SAMPLE MONITORING PROGRAMS

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ABSTRACT:

Reduction of agricultural nonpoint source pollution by implementation of Best Management Practices (BMPs) on a water-watershed basis is being monitored by 21 Rural Clean Water Program (RCWP) projects throughout the United States. This paper serves to briefly describe the Idaho and Florida RCWP projects. In addition, the concept of determining the 'Minimum Detectable Change' (MDC) for trend detection for these monitoring programs is introduced.

A measured change in water quality is statistically significant if it exceeds a value defined in this research as the MDC. Given a particular monitoring scheme, the water quality data and its variability can be used to calculate the MDC required in the geometric mean pollutant concentration over time. The factors affecting MDC are: monitoring design, sampling frequency, duration of monitoring, system variability, meteorological variability, hydrologic variability, temporal variability, spatial variability, and the statistical analysis performed. Methods of MDC calculations and the impact of factors affecting MDC are compared using grab sample monitoring data from two RCWP projects.

Due to the high variability within a year and between years, at least 2 to 3 years of both pre- and post- BMP monitoring data are required to determine if a measured change is real or a function of the unmeasured sources of system variability. The MDC computed from grab sample monitoring data on a water-shed basis ranged from 10 to 66 percent over a ten year monitoring timeframe. Results indicate that adjusting the analytic scheme to account for meteorologic and hydrologic factors can reduce the MDC by 0 to 30 percent.

INTRODUCTION

Agricultural nonpoint source (NPS) pollution is a major environmental concern. Nonpoint sources are defined as diffuse land use activities that ultimately cause degradation of ground and surface water (Novotny, 1988). Agricultural NPS pollution includes pollutant losses in surface runoff and pollutant leaching to ground water.

Agricultural pollutants include pesticides, sediment, nutrients, and bacteria from agricultural cropland, livestock holding grazing areas, and forest harvesting. The impact of NPS is becoming more and more evident as point sources come increasingly under control (U.S. EPA, 1987).

Agricultural NPS can be minimized by the implementation of Best Management Practices (BMPs). Best Management Practices are practices that have been designed to control nonpoint pollution and are socially and economically acceptable (Baker and Johnson, 1983). A large amount of data from edge-of-field studies support the theory that BMPs reduce NPS pollution. In the last 10 years there has been a large effort to substantiate this conclusion at the watershed level. Watershed studies document the cumulative impacts of agricultural practices on regional water quality (Baker, 1988; Baker and Johnson, 1983) and may yield different results from field level studies.

Few large watershed studies of agricultural NPA control effectivenes monitor both land treatment and water quality. Three federal programs have attempted to do so: Agricultural Conservation Programs (ACP), Model Implementation Program (MIP), and Rural Clean Water Program (RCWP). There were eight ACP watershed projects in the 1976 to 1982 timeframe. Seven (MIP) projects were conducted in 1978 to 1982. These were the forerunners of the RCWP. One of the lessons learned from MIP was that a much longer timeframe than 4-5 years was needed to evaluate agricultural NPS control practices on a watershed basis (Humenik et al., 1987). A range of projects sponsored by federal, regional, and state agencies are described by Smolen et al. (1986). These include state 208 projects, 108A, Pollution of the Great Lakes for Land Use Activities Reference Group (PLUARG), state, and U.S. EPA projects. Section 319 of the Water Quality Act of 1987, if funded, will allow additional watershed level NPS projects in each state.

Reduction of agricultural NPS pollution by implementation of BMPs on a watershed basis is being monitored by 21 RCWP projects throughout the United States. The emphasis in project selection and implementation was from the water quality impairment and pollutant control perspective. The RCWP is a 10 year program (1980-1990) with pre-, during-, and post- BMP implementation water quality monitoring. Farmers have 3 to 10 year contracts to implement water quality plans which include BMPs for all critical aread or sources of pollutants on the farm. Funding and administration is a joint effort between USDA, U.S. EPA, state and local agencies.

RCWP is now in its eighth year. The Federal agencies and projects are looking at ways to transform the highly variable water quality data into information. Specific information goals include documentation of agricultural NPS control on a watershed basis, examination of the water quality monitoring designs in terms of their effectiveness in detecting changes in water quality over a 10 year time frame, and application of this information to future watershed level NPS control projects such as those proposed under Section 319 of the 1987 Clean Water Act.

The Minimum Detectable Change (MDC) is defined as the minimum change in a pollutant concentration over a given period of time to be considered statistically significant. The MDC is expressed as a percent decrease relative to the initial geometric mean concentration. To clarify, MDC is the percent change over all years, not a year change, and depends on the number of monitoring years considered. The MDC for a system can be estimated from data collected within the same system or a similar system. A system is defined by the watershed size, water resource and hydrology, monitoring design, pollutants measured, frequency of samples, length of monitoring time, hydrology, and meteorology. The MDC is a function of these system components, the system variability, the statistical techniques and significance level used to analyze the data, the covariates used in the analyses which 'adjust' or 'explain' some of the variability in the measured data, the presence of autocorrelation, the number of samples taken per year, and the variability of the measured observations.

In designing a monitoring system and subsequent methods to detect changes in water quality over time due to land treatment (e.g. BMP implementation) or detect differences between treatments, one would like to increase the precision of statistical analysis by minimizing the error term and the bias. As much as possible, one must account for variability due to other influences in the system (Montgomery and Sanders, 1986). Hydrologic and meteorologic covariates can be used to account for water quality variability.

Measurement and adjustment for climatic variables is important when quantifying the impacts of changes in land treatment/use on regional water quality. In this fashion, the adjusted water quality values are closer to those that would have been measured had there been no change in the climatic variables over time (Spooner et al., 1985).

Water quality grab sample data from the Florida and Idaho RCWP are analyzed in this paper to determine the magnitude of measured water quality pollutant changes required before they can be considered real and not artifacts of system variability. The use of meteorologic and hydrologic covariates to reduce the MDC is examined.

PROJECT DESCRIPTIONS

Taylor Creek-Nubbin Slough RCWP, Florida

The Taylor Creek - Nubbin Slough (TCNS) Basin is located directly north of Lake Okeechobee in southern Florida. The watershed covers 44,550 hectares (110,000 acres) of flat land with generally coarse textured soils. The water table is usually high, and standing water occurs in low areas during the rainy season, May to October. Water flow from the basin enters Lake Okeechobee through a flow control structure, S-191 (Fig. 1).

High phosphorus (P) concentrations in Lake Okeechobee promote eutrophic conditions that impair the use of this resource for water supply, fishing, and swimming. Agricultural NPS pollution has been documented as a significant water quality

problem in the TCNS watershed (Allen et al., 1982). The TCNS Basin contributes 27% of the external P load but only 4% of inflowing water to the lake (Frederico, 1981).

Land use in the watershed is primarily agricultural. Intensive dairy farming is the major agricultural land use. There are 24 dairy barns with approximately 28,000 cows. Other agricultural operations include beef cattle with 56 beef cattle ranches grazing about 25,000 head on improved pastures that are ditched and fertilized. Citrus groves occupy approximately 567 hectares (1,400 acres) and require extensive drainage and irrigation. The main sources of high phosphorus loads in the watershed are thought to be stock animals (dairy cows and beef cattle) excreting while wading in streams to relieve heat stress and runoff from improved pastures and barnyard waste (Stanley et al., 1986). Streambank erosion from animals lounging in the streams is also thought to be significant.

About 25,560 hectares (63,109 acres) have been identified as critical areas needing treatment. This includes all dairy farms, all beef cattle ranches that have been extensively drained by surface ditches, and all areas within one quarter mile of a waterway.

The general treatment strategy was to install BMPs which exclude dairy cows and beef cattle from waterways and to control wastewater runoff from dairy barns. Principle BMPs used are stream protection systems (e.g. fencing), reduction of barn waste by improving water use efficiency and improving effluent disposal with spray irrigation, animal waste management systems, diversion systems, grazing land protection systems, permanent vegetative cover, sediment retention structures, and water control structures. Dairy closures independent of RCWP activities may also affect water quality within the basin. This project has a high level of BMP implementation, most of which occurred in 1985 to 1987.

Grab samples are taken biweekly at 23 stream stations (Fig. 1); some monitored since 1978. Samples are analyzed for total-phosphorus (TP), orthophosphate-P

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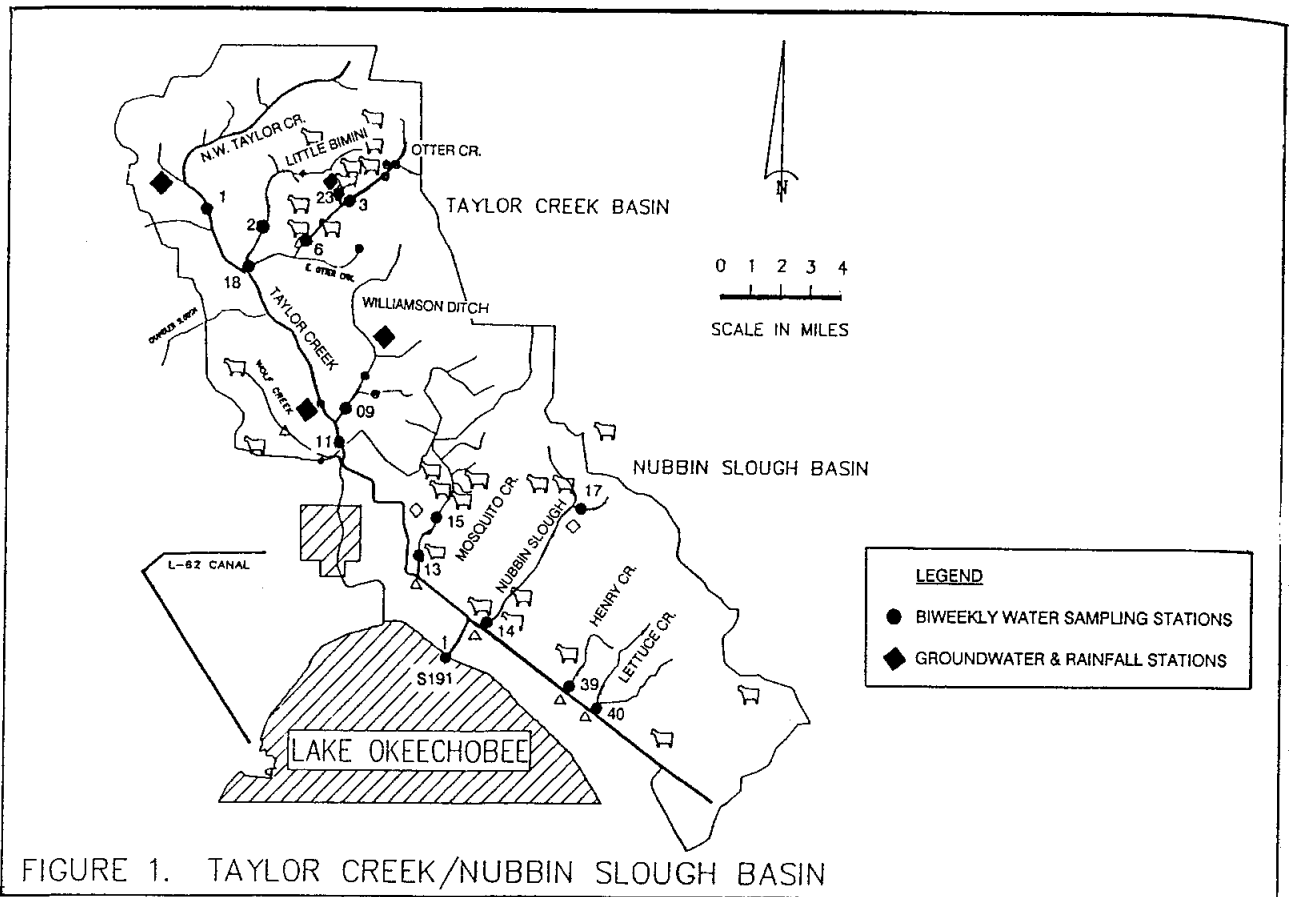FIGURE 1. TAYLOR CREEK/NUBBIN SLOUGH BASIN

Figure 1.   Taylor Creek-Nubbin Slough Basin. Water quality trend stations and ground water wells are indicated (Ritter and Flaig, 1988).

(OP), nitrate-nitrogen (Nitrate-N), nitrite-N, ammonia, total Kjeldahl nitrogen (TKN), pH, conductivity, turbidity (NTU), and color. Flow measurements have been taken at five stations since 1978 and at the remaining stations since 1983. Precipitation and hourly ground water levels have also been monitored at sites in close proximity to stations 01, 03, 06, 09, 11, and 23. Monitoring under the RCWP will continue until 1991. There are some pairs of downstream-upstream monitoring stations to adjust for pollutant concentrations originating above the BMP implementation sites.

Rock Creek RCWP, Idaho

The Rock Creek project, located in south central Idaho, is 18,321 hectares (45,000 acres) with 11,404 hectares (28,000 acres) designated as critical. There are about 350 farm units in the area that produce dry beans, dry peas, sugar beets, corn, small grain, alfalfa, and livestock (Clark, 1975).

Annual rainfall is low and irrigation is required for crop production. Water is supplied to crops primarily by furrow irrigation. Irrigation ditches, which originate from main canals, carry water to individual farms and eventually empty into Rock Creek, which discharges into the Snake River (Fig. 2).

Rock Creek has been reported to have poor water quality. A 1975 report by the Idaho Department of Health and Welfare documented the water quality status of Rock Creek and recommended clean-up of both point and nonpoint sources (Clark, 1975). Major sources of nonpoint pollution in the area are sediment and associated pollutants (i.e. phosphorus and nitrogen) from irrigation return flows. Animal waste is another contributor to the NPS problem. Recreation, fishing, and esthetics are impaired in Rock Creek. In addition Rock Creek delivers a disproportionate load of sediment to the Snake River.

Cropland BMPs include conservation tillage, sediment basins, vegetative filter strips, and management of irrigation return flows.

Monitoring stations have been established on Rock Creek since 1980 and the irrigation tract project is divided into 10 subwatersheds, six of which have been monitored since 1981. The subwatershed stations are located on irrigation ditches, most of which originate at the canals (Fig. 2). Some of the subwatershed stations are positioned in pairs at the downstream and upstream points of the ditches within the subwatersheds, with the downstream stations representing outlets from the subwatersheds to Rock Creek.

Grab samples are taken biweekly during the irrigation season at the Rock Creek stations; the subwatersheds are sampled biweekly at the beginning and end of the irrigation season, which extends April 1 to October 15, and weekly during the middle of the season (mid-May to early August). Samples are analyzed for TP, OP, total suspended solids (TSS), fecal coliform (FC), TKN, and inorganic-N. Instantaneous flow measurements are also taken with each sample.

METHODS

Calculating the water quality concentration change required to detect significant trends requires several steps. The following procedure outlines the steps taken in the analysis performed in this paper. The calculations use the existing grab sample monitoring designs and collected data to determine the MDC. The calculations employ standard parametric statistical techniques which are applied to the complex world of agricultural NPS control watershed level projects.

Step 1. Define monitoring goal - For this paper the goal is to detect a statistically significant change in the annual mean concentration of a pollutant that may be related to land treatment changes.

Step 2. Perform preliminary data inspections to determine if the residuals are distributed independently with a normal distribution and constant variance.
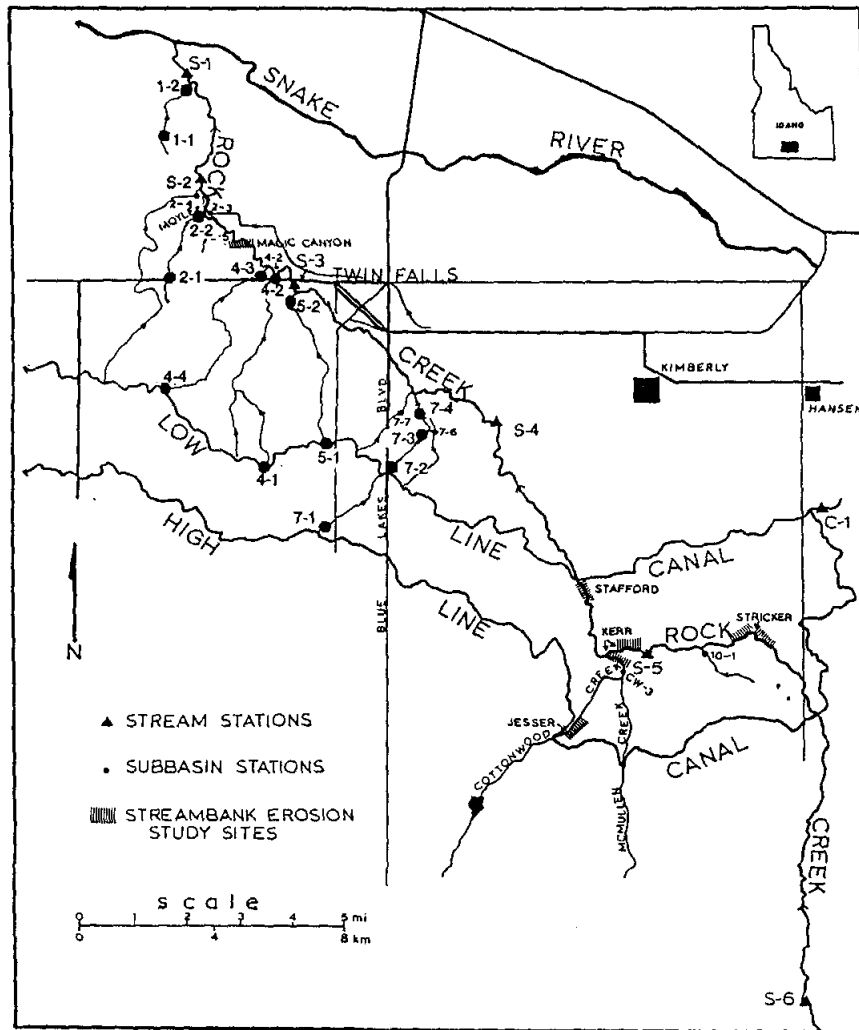
Figure 2.   Map of the Rock Creek, Idaho RCWP project area. Water quality monitoring stations are indicated (Clark, 1988, p. 268).
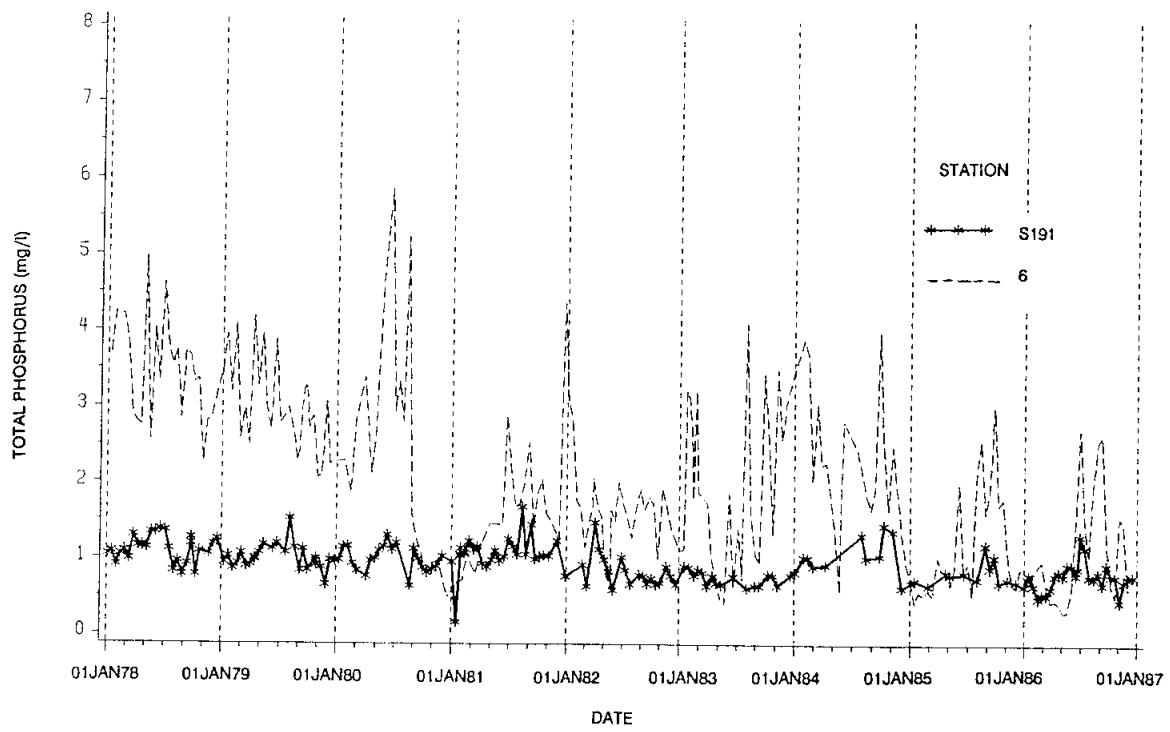
Figure 3.   Total phosphorus concentrations at Station S191 and downstream Otter Creek Station 06.
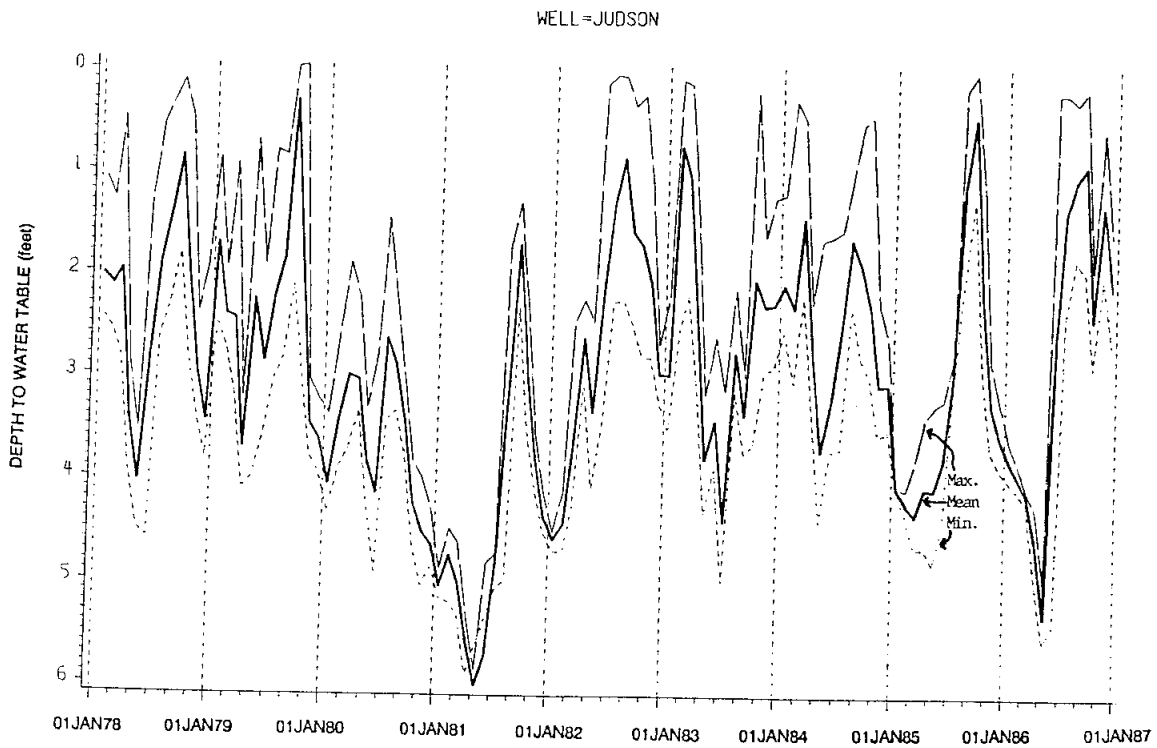Florida RCWP.

Figure 4.   Monthly minimum, mean, and maximum water table depth for the Judson Well Water Gage.
This is in close proximity to water quality monitoring Stations 03, 06, and 23.

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Step 3. Water quality monitoring data were not normal and often did not exhibit constant variance over the data range. A log transformation was used in all the analyses to minimize the violation of these assumptions.

Step 4. The Durbin Watson Test for autocorrelation was performed on the residuals from the planned linear regression models to determine if the concentration measurements were related to previous measurements (SAS, 1984). If autocorrelation is present, the following occur:

a. Standard errors on the coefficients calculated by ordinary least squares (OLS) without paying attention to autocorrelation are not valid;

b. The true standard errors for OLS regression coefficient estimates are not those indicated by ordinary least squares computer programs because ordinary least squares does not take into account the presence of the missing lag variable(s);

c. The true standard errors for generalized least squares (GLS) are exactly what is calculated by statistical computer programs.

d. The true standard errors calculated by GLS regressions which account for autocorrelation are valid (see equation for s_b in step 6 below) and are smaller than those for the true standard errors for OLS. Note that neither the true standard errors for OLS from a model without the autocorrelation term or from the correct autocorrelation model using GLS correspond to the standard errors calculated by ordinary least squares computer programs;

e. The standard errors on the slope calculated by the correct auto-correlation model will often be larger than those incorrectly calculated by ordinary least squares.

Thus, to be truly significant, a change must be sufficiently larger than its true standard error. If autocorrelation is significant, it must be accounted for in the regression models for the appropriate calculation of the standard deviation of the slope over time. Auto-correlation was significant at every station for both the weekly and biweekly grab sample measurements. Therefore, we calculated MDC after correcting for autocorrelation by the use of an autoregressive model of order 1 (SAS, 1984).

Step 5. The MDC was calculated for each station assuming a linear trend over time by linear regression models. The linear regression models estimated from the data were:

a. Log (Variable Y) =
   $b_0 + b_1(DATE) + V_t$

b. Log (Variable Y) = $b_0 + b_1(DATE) + b_2(X) + V_t$

Where V_t is assumed to be generated by an autoregressive process of order 1, AR(1) and X represents a model covariate. The term covariate was used because the explanatory variables are the same as would be used in an analysis of covariance model.

In the Idaho RCWP, upstream concentration was used as a covariate. Adjustment for incoming upstream concentration was used to isolate water quality trends related to land treatment in the watershed between the monitoring stations. Several hydrological and meteorological indexes were developed to use as covariates with the Florida RCWP biweekly grab samples: 1) average water table depth three days before sampling, 2) a weighted average of the last seven days precipitation giving more influence to larger magnitude events closer to the sampling date, 2) upstream TP concentrations; and 4) an indicator variable to separate the wet season (May 15 - October 15) from the dry season. This latter index could be used for all stations and was not limited to those that had upstream monitoring stations, water table depth, or precipitation measurements. Ground water table depth is thought by the project to be a surrogate covariate for the project area hydrology.

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Step 6. The standard deviations on the slope over time from linear regression models were utilized to calculate the MDCs. A significance level of $\alpha=.05$ and a Type II error of $\beta=.5$ were assumed. The standard deviation on the slope is a function of the mean square error (MSE or s^2) estimated by the Yule Walker Method, degree of autocorrelation, number of monitoring years, and sample frequency. The standard deviation on the regression coefficients (e.g. slope) was calculated by generalized least squares using the following matrix operation:

$$s_b = \text{sqrt}(s^2(X'V^{-1}X)^{-1})$$

and MDC' was calculated by:

MDC' on log scale =

$$(N-1)^* t_{(n*N-2)df}^* 365^* s_{b1}$$

where s^2 = the MSE from GLS and is an estimate of σ^2.

s_b = the Px1 matrix containing the standard deviations for the regression coefficients, including s_{b1}, where P = number of regression coefficients in the statistical model.

N = Number of monitoring years.

n = Number of samples per year.

t = One-sided Student's t-statistic ($\alpha=.05$).

365 = correction factor to put the slope on an annual basis because DATE is entered as a Date variable.

s_{b1} = = Standard deviation on the slope.

V = Toeplitz matrix. In an AR(1) model, the i,jth element, $V_{i,j}$, is given by $r|_{i-j}|$, the lag $|i-j|$ sample autocorrelation for cells $|i-j| \geq 1$. The $V_{i,j}$ is 1 for i=j and 0 for $|i-j| > 1$ (SAS, 1984). That is, in the GLS model the variance- covariance matrix does not have 0's on all the off diagonal members as in OLS.

Step 7. To express the MDC calculated above as a percent decrease in the geometric mean concentration relative to the initial geometric mean concentration, i.e. on the original scale, the following formula can be used:

$$MDC = (1 - 10^{-MDC'}) * 100$$

MDC' is the difference between the initial mean value and the mean value at time = N years that is required on the log scale to detect a statistically significant concentration decrease. Therefore, MDC itself (step 7) is a comparison of geometric mean values. Transforming from the lognormal regression to the original scale introduces a bias on the MDC estimate (Gilbert, 1987, pp. 149, 164-168). However, the statistical interpretations are based on the lognormal scale (i.e. MDC') and the transformation back to the original scale in step 7 is used primarily for communication of the results to project personnel. Therefore the bias is not believed to have a significant impact on the results of this paper.

The steps outlined above were tested on water quality monitoring data from two RCWP projects. TP concentrations from 15 of the TCNS, Florida RCWP water quality monitoring stations were examined. From the Rock Creek, Idaho RCWP, 7 subwatershed station downstream-upstream pairs and 1 Rock Creek station pair were evaluated. Pollutants examined in the Idaho RCWP were TSS, TP, OP, and FC.

The pollutant concentrations measured at the water quality monitoring stations were examined visually to establish the magnitude of the water quality problem. Variability in the water table depths and rainfall is also discussed for the Florida RCWP.

MDC was calculated for each station and pollutant. The magnitude of MDC with different pollutants was examined in the Idaho RCWP. Reduction of MDC by the use of appropriate covariates was examined.

Tests for significant changes over time (i.e. changes greater than the MDC) at each station were performed. The significance and direction of the concentration changes are discussed in light of land treatment in each subwatershed.

RESULTS AND DISCUSSION

Taylor Creek-Nubbin Slough RCWP, Florida

TP and OP concentrations measured at the water quality monitoring stations were examined visually to establish the magnitude of the water quality problem. The OP and TP concentrations were of similar magnitude at all stations, indicating that most of the phosphorus is in the dissolved phase. The TP concentrations at the outflow from the project area to Lake Okeechobee are plotted in Fig. 3. Concentrations of TP are scattered around 1 mg/l with an apparent slight decreasing trend over time.

The TP concentrations measured in Taylor Creek (stations 18 and 11) range from 0.25 to 5 mg/l with a majority around 1 mg/l. Northwest Taylor Creek (station 01) has TP values ranging from 0.01 to 1.75 mg/l. This subwatershed has very little dairy activity and is used primarily to raise beef cattle. Williamson Ditch and Lettuce Creek also exhibit moderate TP concentrations ranging from 0.01 to 1.75 mg/l. The remaining subwatersheds exhibit much higher TP concentrations. For example TP ranges from 0.5 to 5.5 mg/l in Otter Creek at station 06 (Fig. 3). TP concentrations at station 23 on Otter Creek are commonly above 10 mg/l, although the total phosphorus load is relatively small due to low discharge. Outlets from the subwater- sheds Nubbin Slough, Little Bimini, Mosquito Creek, and Henry Creek have high TP concentrations, varying around 2 mg/l. The concentration of TP at the project outlet (Station S191) are lower than those in the upstream tributaries. This is probably due to dilution and phosphorus removal mechanisms in the watershed.

High TP concentrations in the tributaries may be related to water table depth and antecedent precipitation (Ritter and Flaig, 1987). By this scenario, when the water table rises to within 2 feet of the land surface, nutrient rich runoff occurs increasing TP concentrations in the surface water. Monthly minimum, mean, and maximum water table depths are depicted in Fig. 4 for the Judson well monitoring station. This station is close to water quality monitoring stations 03, 06,

and 23. The data show large annual variability in water table depths. In addition, a high water table occurs during the wet season from May to October. The relationship between water table depth and TP is significant (r=.35), although the scatter is substantial, implying that water table depth may influence TP concentrations but is not the only factor. The variability patterns in monthly precipitation are similar to those exhibited by water table depth.

The MDC for each of the water quality monitoring stations determined from the variability in the data is shown in Table 1. It should be noted that these MDC values were calculated for the biweekly sampling design and are expressed as a percent change over all years considered. MDC calculated in this fashion is not a yearly value, but a function of the number years monitored. The autocorrelation term was used in all models including covariate models with meteorological and hydrological indexes. Seasonality decreased the MDC values at some stations; seasonality was a statistically significant covariate at stations S191, 11, 18, and 09. The water table depth covariate was significant at all stations where data were available and decreased the MDC at all sites except station 23. The addition of the precipitation covariate was significant only at stations 06 and 23, and was not as effective as the ground water table variable in decreasing the MDC values. Adjustments for these variables should allow for a more meaningful comparison between years with varying amounts of precipitation.

The use of an upstream covariate was statistically significant and decreased the MDC value substantially at the downstream stations 13 and 06, however, this was not the case at station 14. The upstream concentrations represent incoming pollutant concentrations from natural and agricultural sources upstream from agricultural areas where BMPs are implemented.

Relatively small MDC values were obtained for site S191. This may be due to buffering capacity, inertia, or ponding effects at this station. S191 represents cumulative effects from a large watershed. Although the

Table 1. Minimum Detectable Change Required in the Initial Geometric Mean Concentration of Total Phosphorus at Each Water Quality Monitoring Station Over a 9 Year Monitoring Scheme. All data were adjusted for autocorrelation. The MDC is expressed as a percent decrease in models with different covariates. Florida RCWP.

Tributary(Station)	None	Seasonality	Water Table Depth	Precip.	Water Table Depth & Precip.	Upstream Conc.	Water Table Depth & Upstream Conc.
			Percent Decrease				
Henry(39)	54	53	.	.	.	.	.
Little Bimini(02)	54	47	.	.	.	.	.
Lettuce Creek(40)	66	59	.	.	.	.	.
Mosquito Creek(13)	28	28	.	.	.	15*	.
Mosquito Creek(15)	27	28	.	.	.	.	.
Nubbin Slough(14)	25	25	.	.	.	27	.
Nubbin Slough(17)	35	35	.	.	.	.	.
N.W. Taylor Cr.(01)	37	33	32*	33	31*	.	.
L. Okeechobee(S191)	11	10*	.	.	.	.	.
Otter Creek(03)	41	40	29*	40	29*	.	.
Otter Creek(06)	32	31	25*	32*	25*	19*	19*
Otter Creek(23)	50	49	51*	49*	49*	.	.
Taylor Creek(11)	32	28*	27*	29	27*	.	.
Taylor Creek(18)	39	35*	.	.	.	.	.
Williamson Dt.(09)	35	29*	33*	33	32*	.	.

[1] Precipitation and ground water covariates were only used for monitoring stations in close proximity to their measurement.

* The covariate (s) were significant in the regression model ($\alpha=.05$). Where both water table depth and precipitation were covariates, both covariates were significant for all stations examined except stations 01 and 09 where the precipitation covariate did not add significant information to the models.

Table 2. Minimum detectable change (MDC) required in the initial geometric mean concentration of total suspended solids (TSS) at each downstream water quality monitoring station over 8 years with 20 sample per year. Idaho RCWP.

Subbasin (Station)	Upstream Station Covariate	Covariates None	Upstream Conc.
		Percent Decrease	
One (1-2)	1-1	49	29*
Two (2-2)	2-1	52	52
Four (4-2)	4-1	54	48*
Four (4-3)	4-4	68	51*
Five (5-2)	5-1	52	44*
Seven (7-3)	7-1	68	66*
Seven (7-4)	7-2	66	37*
Rock Creek (S-2)	S-4	59	35*

* The upstream covariate was significant in the regression model ($\alpha=.05$).

MDC values may be relatively small, the time to achieve a significant change will not only depend on the amount of effective land treatment, but also on the amount of buffering capacity in the water system at this site. In contrast, first order stream sites such as 23, 39, 40, 02 exhibited high variability in the TP measurements and have relatively high MDC values. It appears that the variability of the measured observations, and therefore the MDC, is a function of several factors including watershed size, land use, hydrology, and meteorology.

Tests for significant changes over time (i.e. changes greater than MDC) were performed. Phosphorus concentrations in Otter Creek decreased significantly. However, there is strong evidence that two dairy closures (in 1981 and 1985) in that subwatershed may be the cause of this trend (Ritter and Flaig, 1987). Data from Mosquito Creek, a subwatershed with intensive BMP implementation, also show a significant decrease in TP. In contrast, increased animal densities and use of animal feeds with high P concentrations appears to have degraded water quality in the N.W. Taylor Creek subwatershed (Ritter and Flaig, 1987).

At station S191, the watershed outlet, an overall decreasing trend in TP concentrations was significant. The project postulates that this trend is largely a function of the dairy closures in the Otter Creek subwater- shed and the large number of BMPs imple- mented in the Mosquito Creek subwatershed. Fencing, manure management, and fertilizer management are thought to be significant practices related to decreasing total phosphorus concentration. It should be noted that the majority of BMP implementation did not occur until 1985, 1986, and 1987, so major improvements may not be documented until a few years of post-BMP data is collected.

Rock Creek RCWP, Idaho

The subwatershed drained by downstream station 2-2 had a median TSS value of 80 mg/l. Upstream station 2-1 is spring fed and very clear (median TSS value, 8 mg/l) and the

major sediment delivery to station 2-2 occurs between stations 2-1 and 2-2. The downstream-upstream station pairs 4-1, 4-2 and 5-1, 5-2 have similar median TSS values at both the downstream and upstream sites (approximately 50 mg/l) implying that no net sediment loading occurs between these two monitoring station pairs.

In contrast, downstream stations 1-2, 4-3, and 7-4 had much higher median values between 275 and 345 mg/l. For two of these subwatersheds (1 and 7), the upstream concentrations were also high implying that the major sediment loading occurs above the upstream monitoring sites. The major sediment loading in subwatershed 4 occurs between the upstream site, 4-4 (median TSS value, 50 mg/l) and the downstream site, 4-3 (Fig. 5).

Downstream station 7-1 had a median TSS value of 165 mg/l with the upstream station, 7-2, having relatively clear water (median TSS value, 35 mg/l). Rock Creek downstream station S-2 exhibited median TSS values of 100 mg/l. The upstream station S-4 was clearer (median value 48 mg/l) (Fig. 6). High TSS in Rock Creek is due to contributions from subwatersheds and stream bank erosion in Rock Creek itself.

The MDC for each of the downstream monitoring station pairs are shown in Table 2. The upstream concentration covariate was significant at all subwatersheds except 2 and reduce the MDC substantially at most stations. Table 3 gives the range and median MDC values for four pollutants. TSS and FC have the most variability between samples and therefore have higher MDC values.

The measured decrease in TSS concentration at the downstream stations was greater than the MDC and therefore statistically significant at all subwatersheds except 7 when no adjustment was made for the upstream concentrations. However, the trends become nonsignificant in subwatershed 1 and at Rock Creek station S-2 when adjustment for upstream concentration was performed.

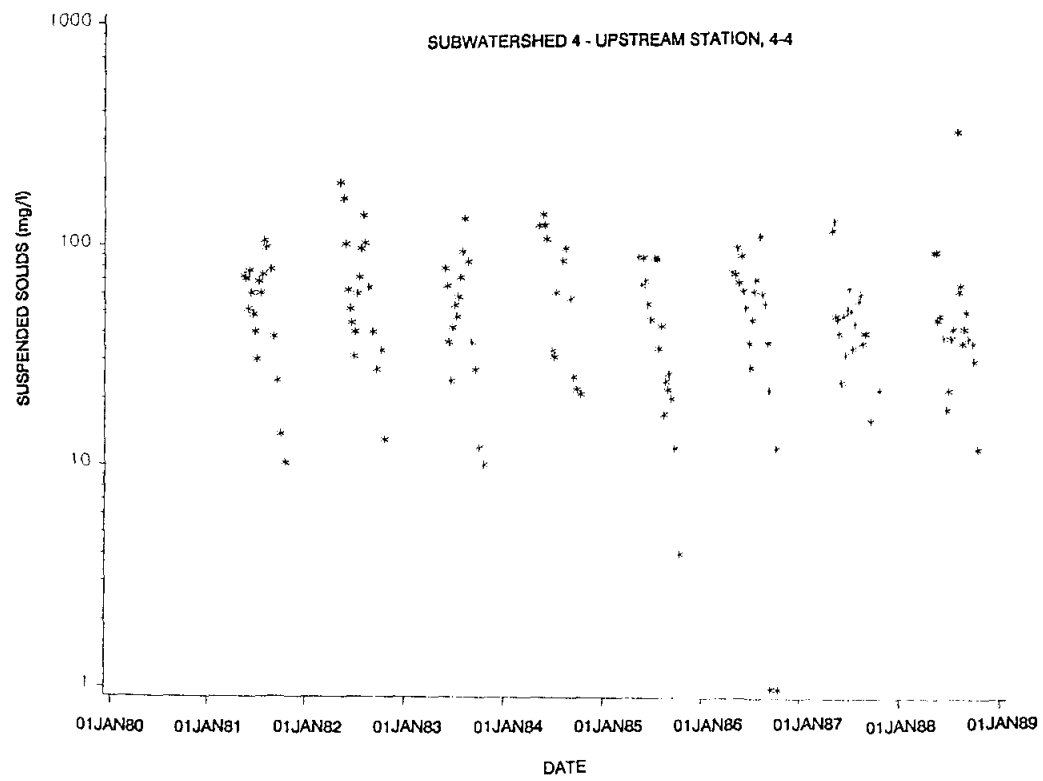There was no apparent relationship between the MDC values and the watershed
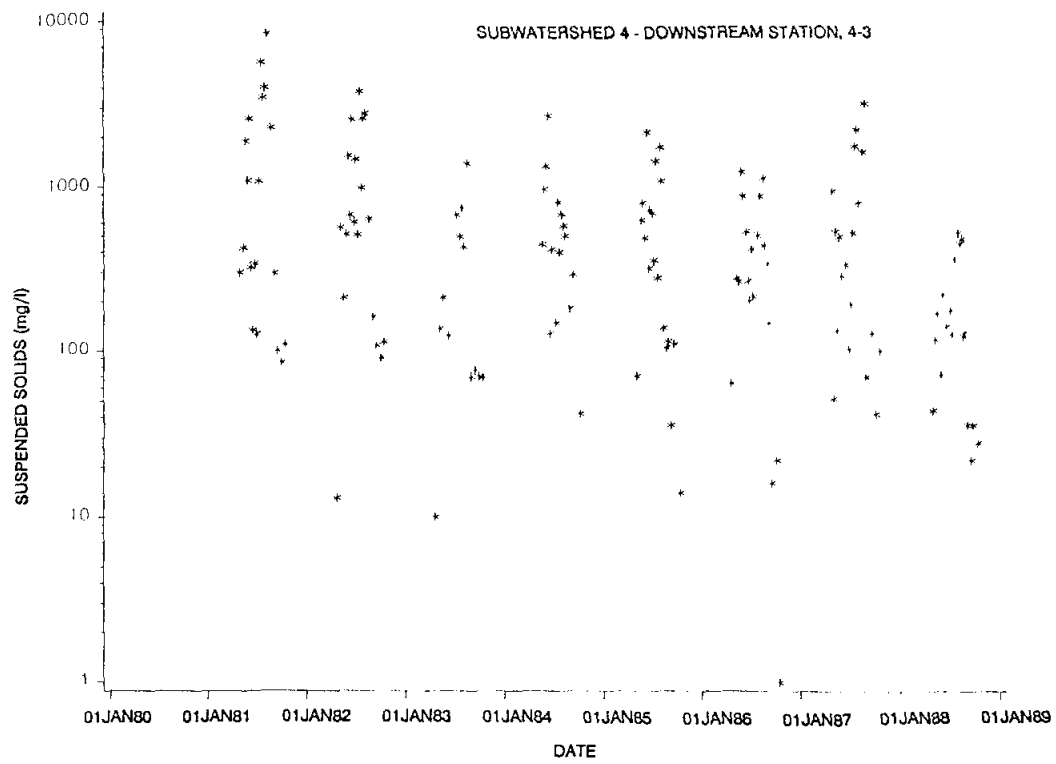
130

Figure 5.   Total suspended solids at downstream-upstream subwatershed monitoring Station pairs 4-4 and 4-3.
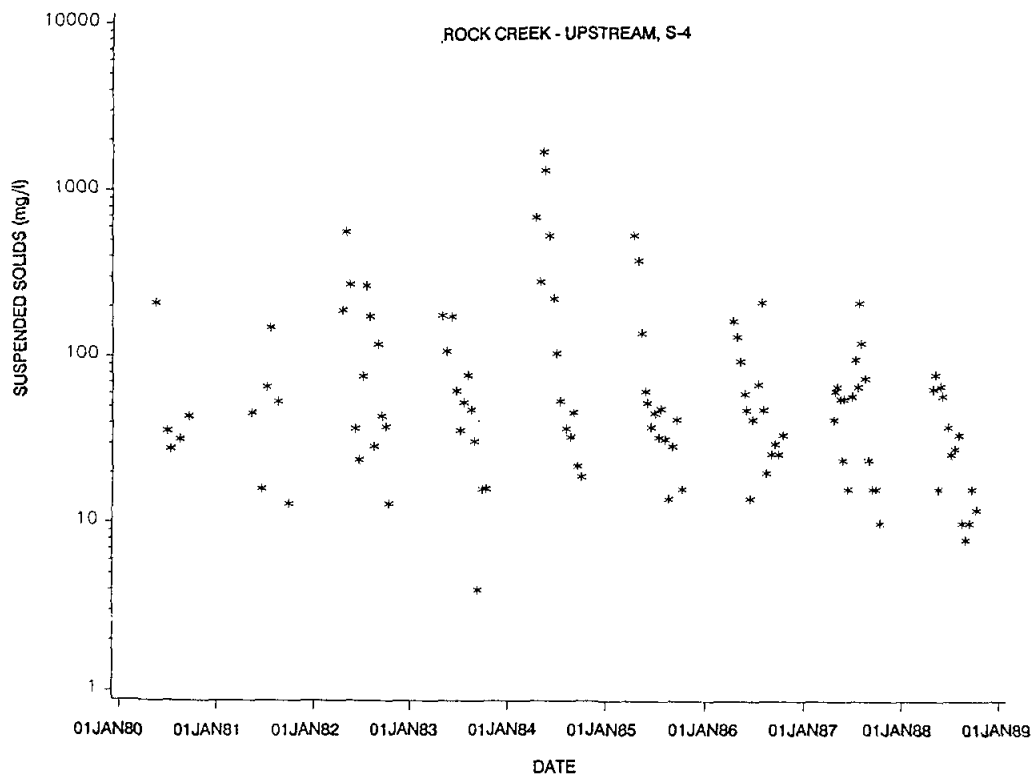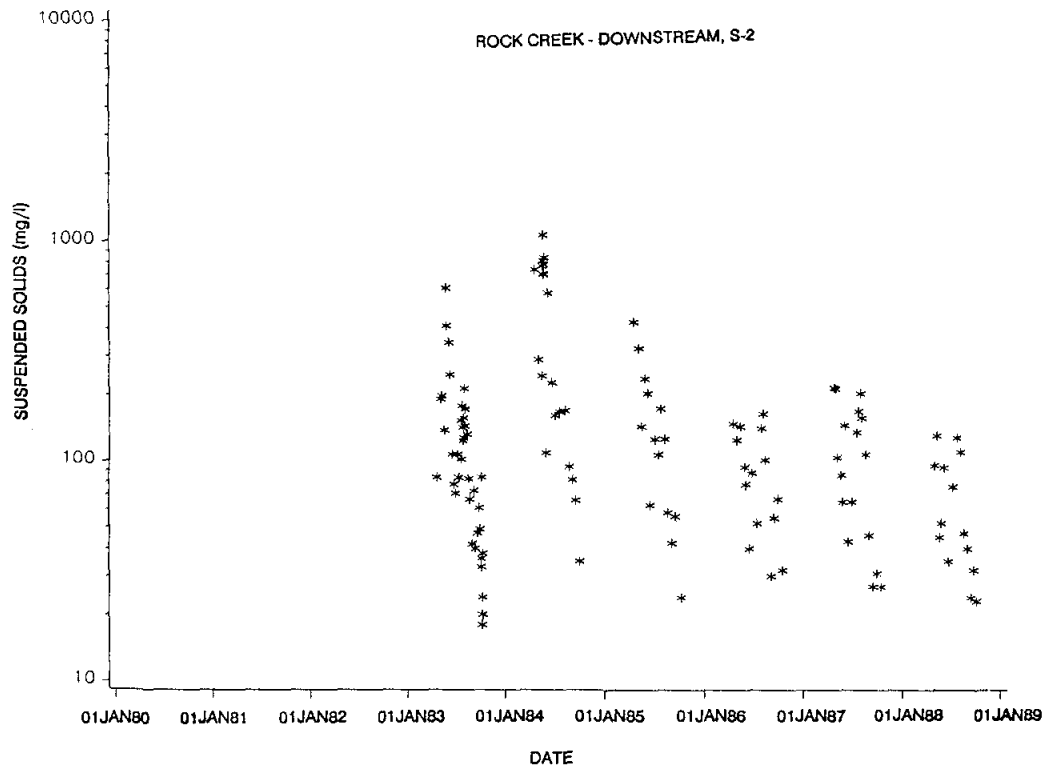
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Figure 6.   Total suspended solids at downstream-upstream Rock Creek monitoring Station pairs S-2 and S-4.

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Table 3. The median and range (in parentheses) of MDC over 8 years at 8 downstream stations for six water quality variables. Upstream concentration were not considered. 20 samples per year. Idaho RCWP.

Variable	MDC (Percent Decrease)
Ortho Phosphate-P	40 (33,43)
Total Phosphorus	43 (32,52)
Total Suspended Solids	56 (49,69)
Fecal Coliform	57 (49,70)

shed size or median TSS concentration. MDC is derived on a log scale and is expressed as a dimensionless percent. Therefore, much of the influence of initial concentration on MDC has been removed by the calculations.

CONCLUSIONS

Water quality monitoring data from the Taylor Creek - Nubbin Slough, Florida RCWP and the Rock Creek, Idaho RCWP agricultural NPS control projects were examined for significant trends in pollutant concentrations. The statistical analysis employed calculation of the minimum detectable change (MDC) required to say with confidence that changes in pollutant concentrations over time were real. The MDCs for TP at the Florida RCWP monitoring stations ranged from 10 to 59 percent after adjustments for precipitation, seasonality and ground water level. MDC was found to be a function of subwatershed size and variability in covariates such as antecedent precipitation, ground water levels, season (wet or dry), and upstream concentrations.

The MDC for TSS at the Idaho RCWP downstream monitoring stations ranged from 49 to 68 percent. After adjustment for upstream concentrations, the MDC values ranged from 29 to 66 percent. The MDC for TSS and FC were much larger than for TP and OP.

There are many confounding factors in water quality analysis and it is difficult to identify and account for all of them. However, by using the MDC, it is possible to evaluate with confidence real changes in pollutant concentrations over time. This technique can contribute to improved analysis of the effectiveness of NPS control efforts. Adjustment for the appropriate meteorological and hydrologic covariates allows for a better assessment of the real BMP impacts on water quality.

Watershed systems are highly variable and require as much as 40-60 percent reduction in pollutant concentrations over 6 to 10 years before statistical trend tests will indicate the

change is significant. RCWP is a 10-year experiment and the projects should be able to document further significant decreases in TP concentrations over time.

The data from the RCWP projects is just beginning to be analyzed and these results should be considered preliminary. On going research includes:

1. Examining the effect of variability between replicates, sampling times, within a day, or within a week on MDC;

2. Pooling across sampling locations and accounting for spatial autocorrelation;

3. Extending the statistical models to ones that allow for a level Pre-BMP period and a linear trend after BMPs are initiated such as a linear plateau model;

4. Test whether transfer functions which relate the response variable to past and present values of covariates would be appropriate;

5. Relate significant water quality changes to land treatment. This is difficult to accomplish in a watershed level study with no true experimental control, but hopefully, correction for the appropriate covariates will help in this attempt.

Agency, or the United States Department of Agriculture.

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DETERMINATION OF SAMPLING FREQUENCY FOR POLLUTANT LOAD ESTIMATION USING FLOW INFORMATION ONLY

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ABSTRACT

Design of monitoring programs for load estimation is often hampered by the lack of existing chemical data from which to determine patterns of flux variance, which determine the sampling program requirements when loads are to be calculated using flux-dependent models like the Beale Ratio Estimator. In contrast, detailed flow data are generally available for the important tributaries. For pollutants from non-point sources there is often a correlation between flow and pollutant flux. Thus, measures of flow variability might be calibrated to flux variability for well-known watersheds, after which flow variability could be used as a proxy for flux variability to estimate sampling needs for tributaries for which adequate chemical observations are lacking. This amounts to a transfer of information between the target variable, flux variance, and an available and related variable, flow variance. Three types of measures of flow variability have been explored: ratio measures, which are of the form x/y, where x is a chosen percentile of flow and y=100-x; spread measures, of the form (x-y)/m, where m is the median flow; and the coefficient of variation of the logs of flows. The ratio and spread measures are scale independent, and thus are measures only of the shape of the distribution. The coefficient of variation is also scale independent, but in log space. Values of these measures of flow variability for 120 Great Lakes tributaries are highly intercorrelated, although the relationship is often non-linear. The coefficient of variation of the log of the flows is also well correlated with the coefficient of variation of fluxes of suspended solids, total phosphorus, and

chloride, for a smaller set of rivers where abundant chemical data allows comparison.

INTRODUCTION

Intensive study of patterns of non-point source transport in a number of Great Lakes tributaries over the last decade has produced a body of information about the behavior of these systems under different flow conditions. This information suggests probable patterns of behavior for less thoroughly studied tributaries in the Great Lakes system, and with increasing uncertainty for the behavior of tributaries outside the Great Lakes system. This paper explores some aspects of information transfer between different attributes of the same tributary, and between different tributaries.

In tributary systems which are dominated by non-point sources of pollution, concentration patterns in the tributary are determined largely by the interaction between the hydrologic cycle and the landscape. Concentrations of most particulate and some dissolved pollutants increase with increasing flow, especially when the flow increase is a result of storm runoff. Concentrations of others may remain approximately constant, or decrease less markedly than flow increases. Flux rates, which are the product of concentration and flow, therefore tend to increase with increasing flow in these systems, in contrast to flux rates primarily from point source inputs, which may be approximately independent of flow. In these non-point dominated systems, the linkage between flow and flux represents information which can be used to estimate fluxes from flows, when

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fluxes are not measured directly (usually, when chemical data are lacking). This linkage also means that, if a river has highly variable flows, it is likely to have highly variable fluxes, and will require a relatively detailed, probably flow-stratified sampling program if precise and accurate pollutant load estimates are sought. It further provides the opportunity, in principal at least, to obtain an initial estimate of sampling needs for load calculations from the flow data alone, in the case where the river is gaged but not monitored chemically.

In the Great Lakes region, the concept of "event responsiveness" has guided research for a number of years. Rivers thought of as event-responsive show large increases in flow during runoff events following storms, whereas stable response rivers have much smaller increases in flow following storms. Soil type is a major factor determining event responsiveness, with event-response behavior typically associated with fine-grained, heavy soils and stable response behavior connected with looser, coarser soils with better infiltration capacity. Land use also has an effect, with agricultural and urban basins typically being more event-responsive than forested ones.

Monteith and Sonzogni (1981) classified the major U.S. tributaries to the Great Lakes into three groups: Event Response, Variable Response, and Stable Response. The classification was intended to reflect the relative difficulty of characterizing loadings, particularly of suspended solids and total phosphorus, from each tributary. Their classification was based on the slope of the regression of suspended solids concentration on flow (Sonzogni et al. 1978); or on flow patterns, soil type and land use, for those tributaries for which concentration data were inadequate or unavailable. Unfortunately, relatively few tributaries had adequate concentration data, so the classification of most tributaries had to be done using these secondary criteria.

Richards (1989a) examined the patterns of flow variability among Great Lakes tributaries, developed and evaluated seven scale-independent, continuous measures of flow

variability, and compared them with each other and with the classification of Sonzogni and his colleagues. In a related work, Richards (1989b) used the flow measures to reclassify the Great Lakes tributaries into event-response groups, updating the work of Sonzogni and Monteith and extending it to the Canadian Tributaries. This current paper demonstrates the potential utility of flow variability measures in planning monitoring programs, and discusses some related aspects of potential information transfer between flow variability and flux variability.

THE MEASURES OF FLOW RESPONSIVENESS

Since flow data are usually not normally distributed (though often approximately log-normal), non-parametric measures were chosen to reflect the variability of the flows. Measures were to reflect the shape of the flow distribution, not its location; for this reason all flow measures were made independent of magnitude of flow. The measures were of three types: ratio measures, spread measures, and an analog of the coefficient of variation using log-transformed flow values. Ratio measures are of the form

$$R = \frac{q_x}{q_{100-x}} \qquad (1)$$

where qx is the (high) flow associated with the xth percentile in the flow distribution, and q100-x is the (low) flow associated with the percentile in the distribution equidistant from the median in the other direction. Three specific ratios were examined by Richards (1989a), based on the percentiles 10/90, 20/80, and 25/75 (referred to as 10R90, 20R80, and 25R75, and collectively "the ratio measures"). These were chosen because the greatest difficulty in sampling has to do with characterizing the extremes of flow, particularly the high flows. Experience with northwest Ohio tributaries indicates that the 25th or 20th percentile is about the cutoff between normal low flow and storm runoff. The more extreme ratio (10R90) was calculated because much of the total discharge

occurs at flows above the 80th percentile (see Baker, 1982, 1988).

The second type of measure is based on the non-parametric analog of standard deviation, the spread. The commonly used fourth spread is defined as the difference between the 75th percentile and the 25th percentile (the "fourths"). A spread can be made scale independent by dividing it by the median. The resulting measure is then analogous to the coefficient of variation of parametric statistics, and is given by

$$S = \frac{q_x - q_{100-x}}{q_{50}} \qquad (2)$$

where notation is as in (1) and q50 is the median flow. Relative spread measures studied by Richards (1989a) were based on the same percentiles as the ratio measures, and are referred to as .5S, .6S, and .8S. A final measure of flow variability is the coefficient of variation of the logs of the flows corresponding to the percentiles: {5,10,15,20,........,80,85,90,95}. This measure, referred to below as CVLF5, is provided in printouts from the standard U.S. Geological Survey (USGS) flow duration analysis, and can be readily calculated from tables provided with flow duration analyses of the Water Survey of Canada. Although it is based on only 19 flow values, it preserves the essence of the distribution properties of the population. Numerical experiments using normally distributed random numbers indicate that the set of 19 flow values has essentially the same mean as the parent population, and a standard deviation which is about 88% of that of the parent population, apparently reflecting exclusion of the tails of the parent distribution. CVLF5 differs from the other measures in being a multi-point measure, reflecting the distribution properties of most of the range of the data more than the other measures do. Like the other measures, CVLF5 is scale independent, but in log space.

Richards (1989a) evaluated these seven different measures of flow responsiveness using data from 118 Great Lakes tributaries, 58 in the United States and 60 in Canada.

Flow indices were found unresponsive to the length of the period of record, if the period of record exceeded five years or so. All measures were highly correlated with each other, although the relationships were often non-linear, especially between measures of different types. The correlation between watershed size and the measures of variability was found to be weak, indicating that other factors such as land use and soil type were more important in determining flow variability, and that the measures were scale-independent not only with respect to flow, but for the most part with respect to basin area as well. The ratio measures, and particularly 10R90, were seen to be highly sensitive to near-zero flows in the lower part of the distribution, and were regarded as less useful for further work than the other approaches.

SAMPLING FREQUENCY FOR LOAD ESTIMATION

A commonly used approach to load calculation involves sampling to characterize the mean daily load, which is then multiplied by 365 to obtain an annual load. This program is often carried out in a flow-stratified fashion, in some cases with estimation of hourly loads, or loads at other intervals more frequent than daily, in the high-flow stratum. The Beale Ratio Estimator (Tin, 1965; Baun, 1982) is commonly used to adjust estimates when observations of concentration are infrequent but observations of flow are complete. In all cases, the sampling frequency (of each stratum, if sampling is stratified) is related to the variance of the daily (or other sampling interval) loads. These loads are usually estimated by the instantaneous flux, which is the product of the measured concentration and the flow at the time of sampling.

This approach to load estimation is among the simplest of the methods which have been used or proposed for use in the literature. It ignores non-normality, autocorrelation, and seasonality. It makes no attempt to take account of relationships between flow and concentration or flux to provide estimates of daily loads on days when concentrations are

not measured. Yet, comparative studies Richards and Holloway, 1987; Heidke, Young, and de Pinto, 1987; Preston et al, 1989) have repeatedly shown it to be unbiased, and consistently among the most precise of the methods evaluated. While not always the best method for a given year and a given tributary, it never fails badly. Its robustness makes it a good choice for a load estimation method when a sampling program is being initiated, and little is known of the behavior of the tributary.

The number of samples needed for load estimation can be estimated, provided that we are willing to specify an acceptable margin of error E for the daily loads, and a probability α of having our estimate be in error by more than E. In that case, the number of samples n_0 can be estimated by

$$n_0 = \frac{t^2 s^2}{E^2} \qquad (3)$$

where s^2 is estimated variance (or mean square error, if the Beale Ratio Estimator is used), and t is the student's t value for the chosen probability (α) and n_0-1 degrees of freedom. Since n_0 is not known, t cannot be determined. The usual approach is to substitute the corresponding value from the normal distribution. This approximation is generally adequate if n_0 is greater than about 30 and the distribution does not deviate greatly from normality (Sanders et al., 1983). For n_0 less than 30, the sample size can be adjusted iteratively.

If the acceptable error is expressed as a proportion p of the mean (or equivalently, total) load,

$$E = p\bar{x}$$

then

$$n_0 = \frac{t^2 (cv)^2}{p^2} \qquad (4)$$

since

$$v = \frac{s}{\bar{x}}$$

As an example, we estimate the sampling frequency for a load estimate which is precise to $\pm 10\%$ (i.e. p=0.1) with a probability a of 0.05 of failing to be within 10%. We assume the estimated coefficient of variation is 0.2432. Then

$$n_0 = \frac{(1.96)^2 (.2432)^2}{.01} = 23 \text{ samples.}$$

Note that $t_{.05}$ for $n_0 = 23$ is not 1.96 but 2.074, so the estimate is a little low. Repetition of the calculation using 2.074 instead of 1.96 gives $n_0 = 25$; further iteration does not change the sample size.

Formulas 3 and 4 assume that n_0 is small compared to N, the total number of possible observations (e.g., if the population is daily loads, N=365). Cochran (1977) suggests 5% to 10% as a practical definition of "small compared to". If this condition is not satisfied, then the estimated sampling size may be revised (Cochran, 1977) using the finite population correction

$$n = \frac{n_0}{1 + \frac{n_0}{N}} \qquad (5)$$

Note that n is always less than the smaller of n_0 and N. The choice of whether to apply the finite population correction in the case of load estimation is not clear, since the population units represent arbitrary divisions of a continuous process of pollutant flux, the time integral of which is the true load. While there are only 365 daily loads in a (non-leap) year, there are an infinite number of possible instantaneous estimates of each daily load.

FLOW VARIABILITY AS A PROXY FOR FLUX VARIABILITY

One frequently encountered difficulty in the design of monitoring programs is that there are little or no concentration data from which to construct an initial estimate of load variance for use with formula 3. In this instance, one can estimate the variance from the expected range of daily loads using

$$S^2 \approx \left(\frac{RA}{4}\right)^2$$

as suggested by Sanders et al (1983), guess at the sampling frequency, or just not do the design at all.

While concentration data may be scarce or non-existent, flow data are usually available for important tributaries. Thus one possible use of the measures of flow variability would be to estimate flux variance. Since the measures of flow variability are scale independent, they would be used to estimate the coefficient of variation, which would be used with formula 4.

To examine this possibility, the coefficients of variation were calculated for the daily loads of suspended solids, total phosphorus, and chloride, for ten tributaries of Lakes Erie and Ontario: the Raisin, Maumee, Sandusky, Cuyahoga, Genesee, Oswego, and (New York) Black Rivers; and Honey, Upper Honey , and Rock Creeks. They range from among the most responsive to solidly stable, and include the smallest and next-to-largest tributaries in the overall group studied by Richards (1989a and b). The results for suspended solids are typical and are represented in Figure 1. For each chemical parameter, CVLF5 was the best predictor of the coefficient of variation of the daily loads, and the relationship was best expressed using a logarithmic model. The equations of best fit are given in Table I. Table II lists sampling needs for each river and each parameter, for a=0.05 and p=.2, as calculated using the actual coefficient of variation of daily loads, and as calculated using the coefficient of variation estimated from the relationship in Table I. These results are also shown in Figure 2. The agreement is sufficiently good to demonstrate the potential utility of this approach for the initial design of sampling programs.

Certainly, when the alternatives are to guess at an appropriate number of samples, use an estimated range to estimate a variance, or not attempt to evaluate the sampling frequency at all, the use of flow variability to estimate flux variability offers a useful alternative or supplementary approach.

In principle, flow-based estimates of flux variability could be used in other formulas for sample size estimation, including, with proper modifications, flow-stratified sampling programs. Load estimators which are concentration dependent would have sampling frequencies dictated by the variability of concentrations rather than daily loads. It is not known how well flow variability would predict concentration variability.

Other related uses of flow variability can be readily imagined. Richards (1989b) used the flow variability measures to classify the Great Lakes tributaries and create a map of regions of different variability. Flow variability could be used to allocate samples among stations in a network design problem. Sampling frequency estimates based on flow variability could be used to retrospectively evaluate the adequacy of past monitoring programs. This could be a valuable adjunct to examining the monitoring data itself: in a strongly event-responsive tributary, a grossly inadequate monitoring program may sample too infrequently to even "see" the variance of the system, and give the false impression that it is doing an excellent job, but the much more frequent flow data would suggest otherwise.

CONCLUSIONS

In load estimation programs which use load-dependent estimators, sampling frequency is a function of the variance of the daily loads. The magnitude of this variance is generally unknown when the monitoring program is designed. Measures of flow variability, particularly CVLF5, showed good (non-linear) correlation with the variance of the daily loads of suspended solids, total phosphorus, and chloride on 10 Great Lakes tributaries covering a wide range of flow responsiveness. In the absence of direct information about load variance, initial sampling frequencies for load estimation can be developed from flow information alone.
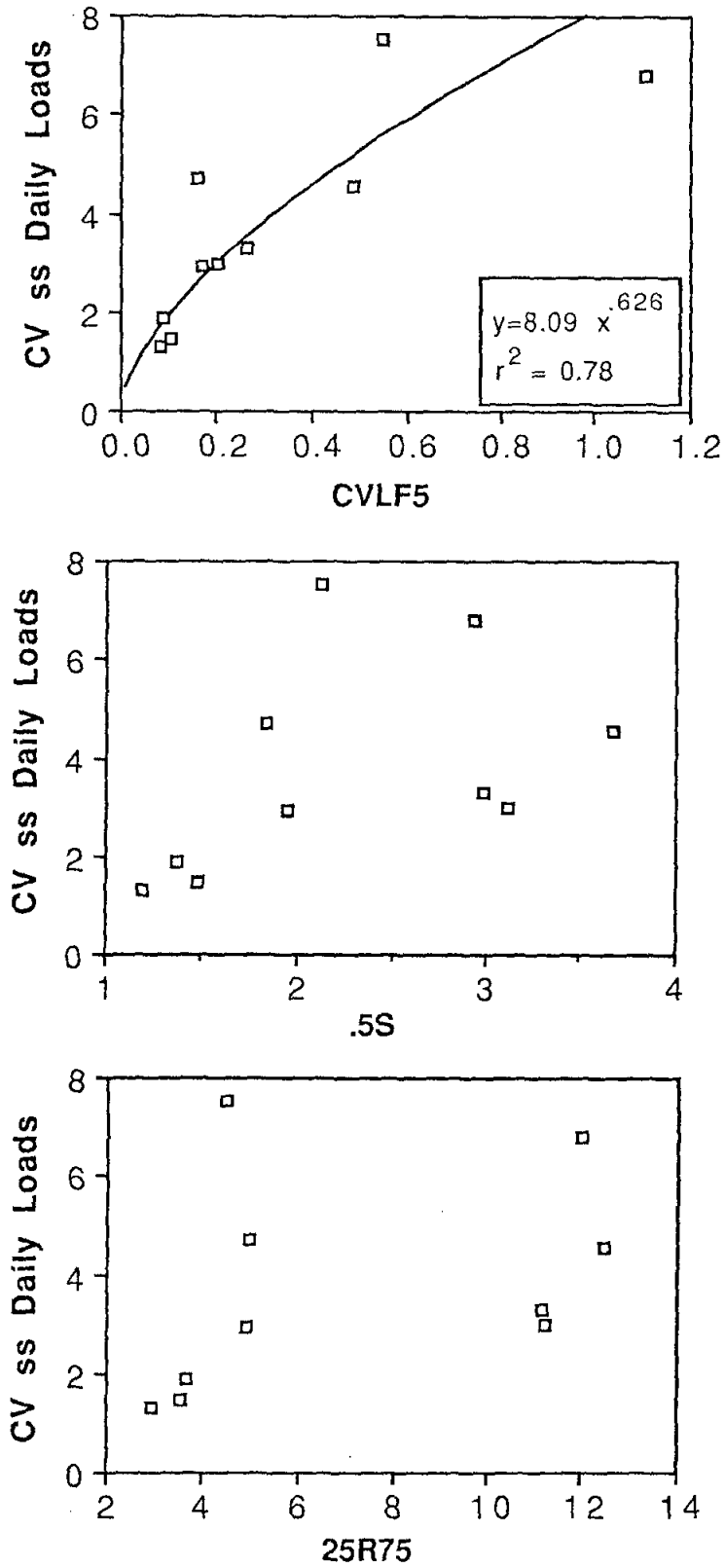
ACKNOWLEDGMENTS

Figure 1. Relationships between the coefficient of variation of daily loads for suspended solids and selected measures of flow variability.

Table I. Relationships between the coefficient of variation (cv) of daily loads and the measure CVLF5 (see text) for 10 tributaries to Lake Erie and Lake Ontario.

Parameter	Equation	r^2
Suspended solids	$cv = 8.09 \, (CVLF5)^{.6259}$	.781
Total phosphorus	$cv = 5.82 \, (CVLF5)^{.5976}$	.887
Chloride	$cv = 2.84 \, (CVLF5)^{.7074}$	.686
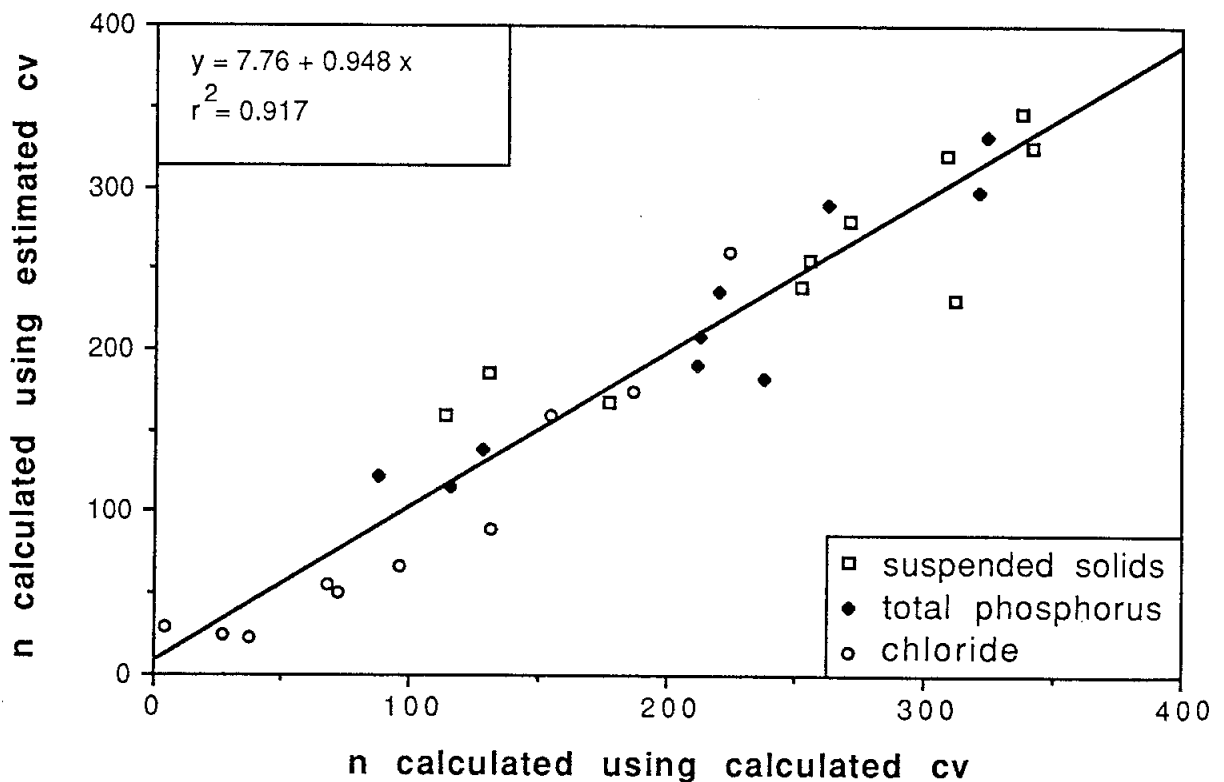
Figure 2. Results of predicting sampling needs from estimated coefficients of variation, for three parameters on 10 rivers. Data are in Table II. Values of n along the horizontal axis are calculated from the observed coefficient of variation. Corresponding values on the vertical axis are calculated from coefficients of variation estimated from the formulas in Table I. The regression results shown are calculated on the aggregated data for all three parameters.

Table II. Comparison of estimated and actual coefficients of variation and resulting sample size estimates. Estimated coefficients of variation were derived using the formulas in Table I, and sample size estimates were calculated according to formulas 4 and 5 in the text.

Parameter and River	Coefficient of Variation: Actual	Estimated	Sample size estimated from: Actual cv n_0	n	Estimated cv n_0	n
Suspended Solids						
River Raisin	2.907	2.691	812	252	696	239
Maumee River	2.974	2.978	850	255	852	256
Sandusky River	3.298	3.528	1045	271	1196	280
Honey Creek	4.544	5.169	1984	308	2566	320
U. Honey Creek	6.782	8.631	4418	337	7155	347
Rock Creek	7.515	5.567	5424	342	2977	325
Cuyahoga River	4.684	2.558	2108	311	629	231
Genesee River	1.452	1.989	203	130	380	186
Oswego River	1.887	1.790	343	177	308	167
Black River	1.308	1.725	165	114	286	160
Total Phosphorus						
River Raisin	2.278	2.035	499	211	398	190
Maumee River	2.299	2.242	508	212	483	208
Sandusky River	2.397	2.635	552	220	667	236
Honey Creek	3.122	3.794	937	263	1383	289
U. Honey Creek	5.498	6.191	2904	324	3682	332
Rock Creek	5.274	4.073	2672	321	1594	297
Cuyahoga River	2.651	1.939	676	237	362	182
Genesee River	1.432	1.525	197	128	224	139
Oswego River	1.089	1.378	114	87	183	122
Black River	1.327	1.331	170	116	171	116
Chloride						
River Raisin	0.932	0.819	84	68	65	55
Maumee River	1.165	0.918	131	96	81	67
Sandusky River	1.458	1.111	205	131	119	90
Honey Creek	1.665	1.712	267	154	282	159
U. Honey Creek	2.450	3.056	577	224	897	260
Rock Creek	1.986	1.862	379	186	333	174
Cuyahoga River	0.963	0.773	90	72	58	50
Genesee River	0.201	0.582	4	4	33	30
Oswego River	0.548	0.516	29	27	26	24
Black River	0.648	0.495	41	37	24	23

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METHODOLOGY FOR THE PLANNING AND OPERATION OF A WATER QUALITY NETWORK WITH TEMPORAL AND SPATIAL OBJECTIVES: APPLICATION TO ACID LAKES IN QUÉBEC

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ABSTRACT

In this paper, we propose a methodology for planning and running a water quality monitoring network. Here, this methodology has been applied to establish a network for detecting trends in the acidification of lake waters in Québec. This has been made possible by an appropriate use of spatial and temporal available information. The spatial information was obtained through the use of multivariate analysis (Correspondence Analysis and Cluster Analysis) on data coming from a lakes survey in southern Quebec in 1983. It has been possible to divide the study area into five homogeneous zones by imposing a neighborhood constraint in the cluster analysis. The spatial density of stations by zones is calculated by the use of the stratified random sampling theory with optimum allocation. The temporal information comes from an analysis of a long data series measured at Lake Laflamme (1982-1987). From the analysis of the autocorrelation function on stationary series, a sampling frequency is determined, which is optimal for detecting significant trends in a reasonably long period of time. A spatio-temporal optimisation procedure is then proposed which involves developing a few sampling plan scenarios with various proportions of emphasis on spatial land temporal components.

INTRODUCTION

The Québec area, located on the precambrian shield, has often been identified as one of the most sensitive regions to acidification (Altshuller and McBean, 1979; 1980; Harvey et al., 1981; Shilts et al., 1981; Lachance et al., 1985). Lakes surveys done throughout Québec have shown some evidence of acidification in the aquatic ecosystems by acid precipitation (Lachance et al., 1985; Dupont and Grimard, 1986; Dupont, 1988). A close relationship has been observed between the sulfate concentration in the precipitation and lake waters, which indicates how important atmospheric transport is on the chemical composition of surface waters.

Because of the threat to aquatic ecosystems from this pollution problem and the fear of the long term consequences of an increase or a reduction in emissions of the pollutants that cause acidity, Environment Canada has established a monitoring network to detect trends in the acidification of surface waters in the province of Québec (Haemmerli et al., 1984).

The spatial aspects of this monitoring network were planned using the analysis of the data base from a survey conducted by Environment Canada during the winter of 1982 on 158 lakes (Bobée et al., 1983). The sampled region is located on the Canadian Shield, north of the Saint Lawrence river, between the Ottawa river and the Saguenay river. The planning of the temporal aspects of the monitoring was based on theoretical considerations and on a summary analysis of an available time series on a calibrated watershed located in the region under study (Bobée et al., 1983). The effects of atmospheric pollutants on aquatic ecosystems

have been under study ever since 1981 at the Lake Laflamme watershed located in the Boreal Forest (Forêt Montmorency) 80 km north of Québec city (Papineau, 1983). Weekly samples have been taken in order to monitor the temporal variability of the quality of the lake water.

This paper reconstructs the steps used to create and implement a network to detect acidification trends. The actual steps in the process we set up were based on highly advanced statistical methods and on supplementary data not available at the time Environment Canada established its network. More specifically, this paper demonstrates how an adequate use of available information can lead to a rational and optimal design of a sampling plan whose purpose is the study of both the spatial and temporal aspects of an environmental problem.

GENERAL CONCEPTS

The different steps used in the acquisition of water quality data follow the same objective process, regardless of the difficulty of the problem to be solved (Wilson, 1974; Sanders et al., 1987; Sherwani and Moreau, 1975; Bobée and Sasseville, 1978). Because of the complexity of natural aquatic systems and the difficulty in evaluating changes resulting from anthropogenic activities, which are sometimes very subtle, special attention must be paid to the planning of each step in the creation of a data acquisition network. The best procedure when gathering information is to have well-defined objectives. That is, they must be clear enough to allow for the conception of an adequate sampling plan and an optimal acquisition of information, subject of course, to available resources. The many steps in the planning of a water quality data acquisition network are illustrated on Figure 1.

As shown in Figure 1, the planning activities include several steps ranging from the definition of the objectives up to the use of the information. Our study deals only with the essential steps that include the use of available information and the consideration of available resources and existing constraints in the design of a sampling plan.

The detection of changes in the acidification of surface waters must be possible under a range of acid atmospheric inputs and take into account the acid buffering capacity of the watersheds. Consequently, the trend detection operation includes both a temporal and spatial analysis (improvement or degradation of water quality at a specific site and extension or recession of affected areas). The two components of this analysis can conflict when available resources are limited, as time trends detection implies a high frequency sampling at a limited number of stations. On the other hand, spatial trend detection requires a high density network to monitor the spatial variability and to control the regional representativity of temporal stations.

Since these two components are conflicting, two distinct sampling plans are needed: one for spatial aspects and the other for temporal aspects. The planning of these two phases is essential and cannot be realized without a knowledge of the spatio-temporal variability of the water quality parameters selected to meet the objectives of the network.

SPATIAL ASPECTS

Spatial Variability Analysis

An analysis of the spatial variability is made using available data in order to subdivide the future network area into a number of homogeneous zones called strata. These strata are determined on the basis of their homogeneity in relation to a set of water quality variables selected to meet the network objectives (that means trend detection in acidification).

The water quality variables considered for this spatial analysis are pH (measure of water acidity), alkalinity (indicator of the buffering capacity of acid inputs), sulfate concentration (indicator of the aggression level by atmospheric sulfur inputs) and the sum of calcium and magnesium concentrations (characterizing the global mineralization). These four chemical variables were selected because they offer high-information content on the sensitivity or the acidity level of the lakes.
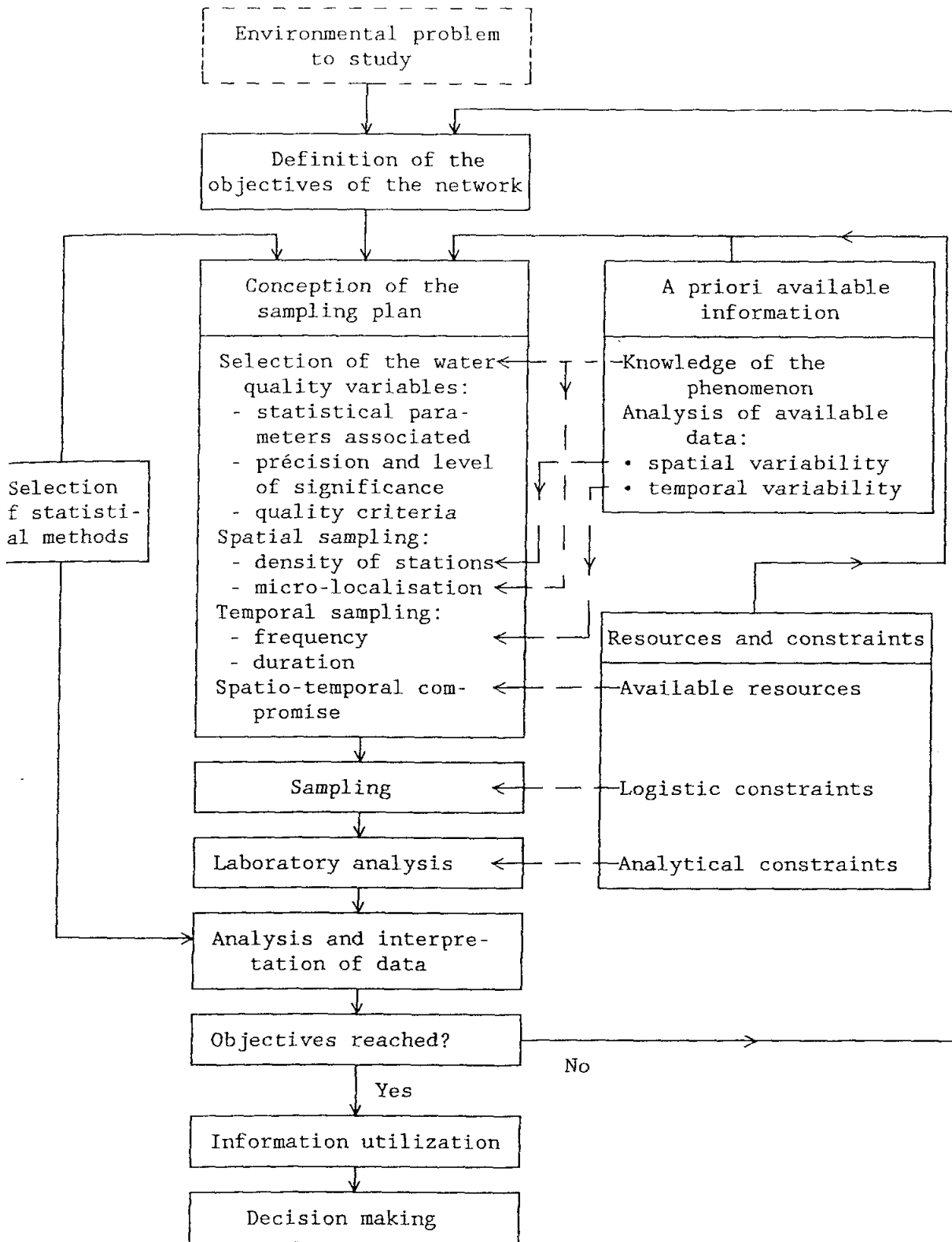
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Figure 1. Diagram illustrating the different steps in the planning of a data acquisition network (After Haemmerli *et al.*, 1984).

The multivariate methods used were correspondence analysis (CA) and ascending hierarchical classification (AHC) (Lebart et al., 1984; Jambu and Lebeaux, 1983). The combined use of these two statistical techniques have led to many applications in water quality data analysis (Lachance, 1988; Bobée and Lachance, 1984; Lachance and Bobée, 1982; Lachance et al., 1979).

Correspondence analysis was developed principally for the analysis of contingency tables analysis and cannot be directly applied to the original data. A binary coding of data is then used. Let X be a (I x Q) table with I observations (stations) as lines and Q variables as columns. On each variable q, we define J_q categories (variation intervals), each one to include a number of observations. Each observation X_{iq} is coded 1 or 0 depending on its presence in or absence from the category. The new coded table k now has I lines corresponding to I observations and J (Σ J_q) columns corresponding to Q variables separated in J_q categories.

For the present application, we decided to define for each variable five categories with an approximately equal number of observations (J_q = 5; q = 1,...,4). Therefore the analysed table has 158 lines corresponding to the 158 surveyed lakes and 20 columns corresponding to four variables, each one separated into five categories.

With this application of CA, it is possible to explain 20.1 and 15.1% of the total variability on the first two principal axes. Inspection of the position of the "category points" on the plane formed by axes 1-2 (Figure 2A) shows that pH, alkalinity and Ca + Mg have a similar variation, whereas the sulfate variable behaves differently. Indeed, when polygonal lines are drawn to join the ordered items, we observe a similar course for these three variables. As for sulfate, the different course is caused mainly by the proximity of low sulfate values to the intermediate values of the three other variables.

Points representing the categories defined for alkalinity, pH and Ca + Mg are distributed as a parabola. It should be

remembered that this type of course, called Guttman effect, is obtained when the phenomenon is mainly unidimensional (Benzécri and coll., 1976). This type of representation indicates that water mineralization, described chiefly by alkalinity, pH and Ca + Mg, is a space continuum phenomenon of the entire region studied.

By means of AHC, five classes of lakes were determined using the distances calculated between the coordinates of the points on the first eight factorial axes. Figure 2B shows the projection of the centres of gravity of the five classes on the same graph with the points representing the categories defined for the variables. In order to be able to picture the dispersion of the cloud corresponding to each of the five classes of lakes (see Figure 2B), the groups of points are shown using inertia ellipses, calculated according to Grelet and Lebeaux (1980). The size of these ellipses shows that the dispersion of each of these clouds is comparable. The absence of superposition confirmed that these five classes of lakes constitute quite distinct groups.

The results of the classification are arrived at by examining proximities between "category points" and the centres of gravity of the classes of lakes. According to the barycentric property of CA, the distance between a category point and a class of observations characterizes the degree of importance of this point in the formation of the class. If we inspect Figure 2B, we see that class E is characterized by high sulfate values (SU5). It is also possible to characterize lake classes more objectively by calculating the contribution of each category point to the position of the centre of gravity of the class in the factorial space. Details of this procedure are given by Lachance (1988).

By examining the information in Figure 2B, it is clear that the points characterizing each of the five classes are the categories defined for the alkalinity, calcium + magnesium and pH. Except for point SU5 which characterizes class E, sulfate is a less determinant variable.

By reporting the class of each lake on the map of the region being studied, we can

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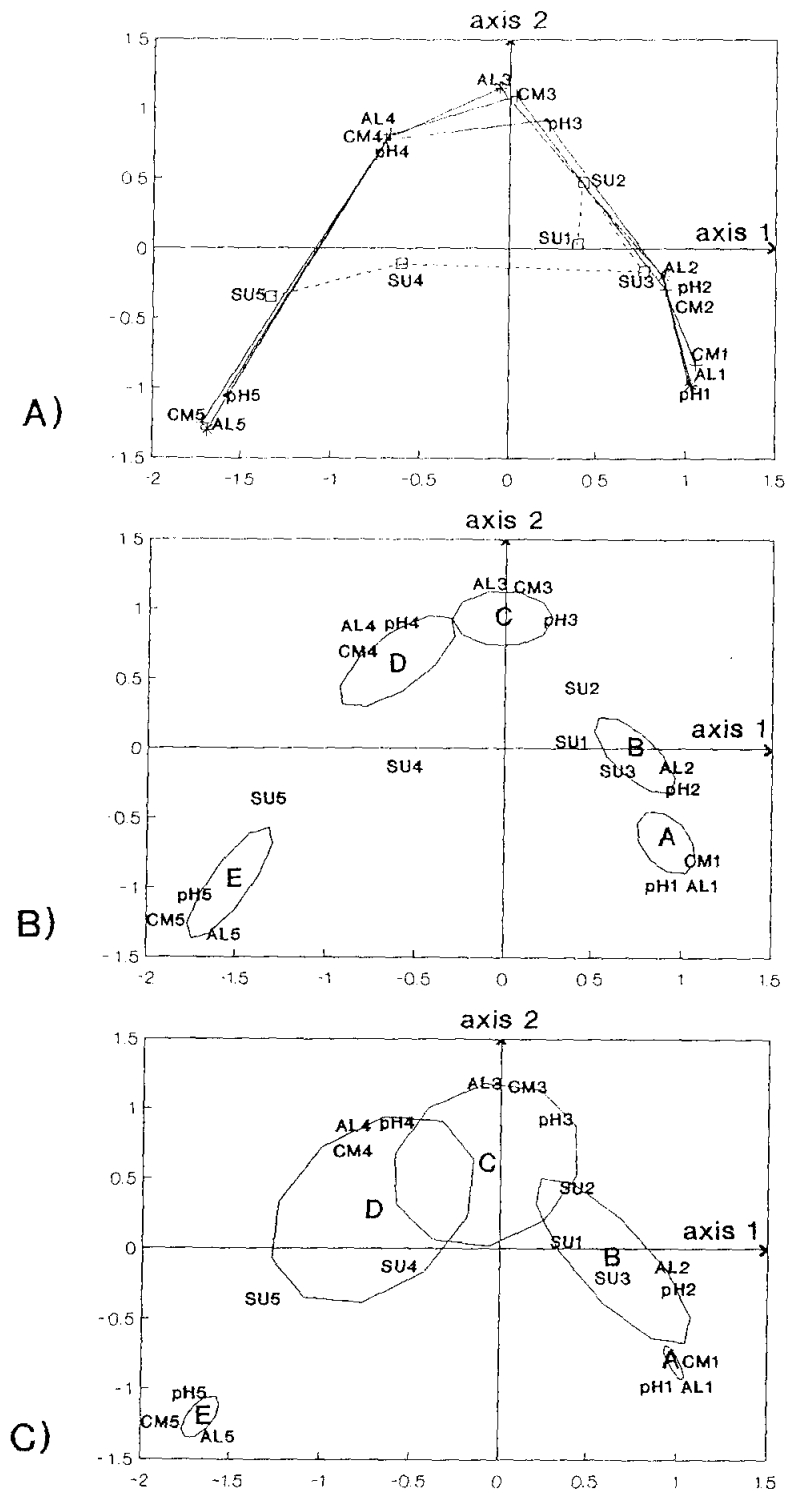
igure 2.   Representation, in the plane formed by the two first principal axes, of:

A) the "category points";

B) the classification of "lake points" without constraint;

C) the classification of "lake points" with a contiguity constraint.

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check whether or not these five classes delineate geographic zones. During the first step of this study, five geographic zones were identified using this method and the supplementary information on the physiographic characteristics of the territory (Bobée et al., 1983). This method is particularly precarious when we find neighbouring lakes belonging to different classes in the same area.

In order to obtain more objective zoning, a contiguity factor was introduced as part of the classification method. With this technique (Lebart, 1978), stations are automatically partitioned into geographically neighbouring classes; these groupings are still made on the basis of similar characteristics for the chemical variables considered. Therefore, to use this method, a contiguity matrix has to be prepared giving the most neighbouring points for each lake. Thiessen polygons are then drawn for each lake (Lachance, 1988). Later, two contiguity notions were defined. A lake is identified as contiguous to another lake when the two have either a common polygon side or a common polygon vertex or side. The latter classification was retained here (Figure 2C).

By using a contiguity constraint, there is an important dispersion increase for classes B, C and D, and a decrease for classes A and E. The larger intra-class dispersion for B, C and D can be explained by the fact that this method sometimes requires that lakes with very different characteristics be grouped together because of their neighborhood. The five geographic zones obtained with this method are shown in Figure 3. The new zones correspond roughly to the zones delineated by Bobée et al. (1983). However, they are now obtained in a more objective fashion.

Spatial Optimisation

The planning of the spatial sampling essentially consisted in determining a density of stations per stratum in the region. To determine this density, we used stratified random sampling with optimum allocation. This method has the advantage of taking into account, for each stratum, the variance of the variable considered, the number of lakes and the sampling cost. If our hypothesis is that the unit sampling price is the same for each stratum, the number n_i of stations per stratum i is given by the following equation (Cochran, 1977):

$$n_i = n \frac{N_i \, s_i}{\sum\limits_{i=1}^{n} N_i \, s_i} \tag{1}$$

where n = total number of stations to be allocated among the different strata;
N_i = population of stratum i;
s_i = standard deviation of the variable for the stratum i.

Table 1 shows the results of the application of this equation for each of the four chemical variables: alkalinity, Ca + Mg, pH and SO_4. We thus obtain four spatial sampling plans (one for each variable). A compromise may be obtained by calculating the arithmetic average of the number of stations for each stratum. This value is not optimal for each variable, but is the best acceptable according to the objectives.

TEMPORAL ASPECTS

Temporal Variability Analysis

To determine the sampling frequency and the duration of the operation of a network needs to have an "a priori" knowledge of temporal variability. Available data for temporal variability analysis came from Lake Laflamme, located inside the studied region (latitude and longitude of 47°19' et 71°07' respectively). Weekly measurements of physico-chemical variables were available for the lake for a period of eight years (1981-1988). This lake meets all the selection criteria used for the survey of the lakes in the region. Because of the physico-chemical may be seen as belonging to zone A (Figure 3).

For the analysis of the time aspects, we continued to consider the four following physico-chemical variables: alkalinity, sulfate,

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TABLE 1: Sampling of spatial variability: number of lakes, standard deviation and number of lakes to sample.

parameter		stratum				
		1	2	3	4	5
number of lakes per stratum (N_i)		104	614	217	176	81
standard deviation[1]	alkalinity	9.0	41.5	95.6	166.3	572.9
(s_i)	Ca + Mg	15.1	42.6	74.8	164.9	534.5
	pH	0.28	0.40	0.38	0.52	0.42
	sulfate	17.7	19.9	12.6	30.2	73.5
number of lakes[2]	alkalinity	1	20	17	24	38
to sample	Ca + Mg	2	22	14	25	37
(n_i)	pH	6	51	17	19	7
	sulfate	7	43	10	19	21
	compromise	4	34	14	22	26

1 Units are given in μeq/L except for pH which is given in units of pH.

2 Total number of lakes to sample is fixed at 100.

TABLE 2: Number of samples per year according to the sampling saturation level.

saturation level n^*/n^*_{max} (%)	alkalinity	calcium + magnesium	pH	sulfate	compromise
50	3	5	7	5	5
60	4	8	8	7	7
70	5	11	11	10	9
80	7	17	15	14	13
90	13	28	25	23	23

Figure 3.   Studied region with the five geographical zones delineated by the application of hierarchical classification with a contiguity constraint.

calcium + magnesium and pH. The temporal evolution (for the period 1982 - 1987) of these four variables is illustrated in Figure 4. The alkalinity and the sum of calcium + magnesium concentrations show very pronounced cyclic variations related to the annual hydrological cycle. There is a sudden decrease in the spring and a gradual increase during the summer and autumn. Sulfate and pH seem to follow an increasing trend, whereas alkalinity, in spite of an important seasonal variation, exhibits a decreasing trend.

Temporal Optimisation

Since the main objective for this network is to determine a temporal trend, temporal optimisation may be seen as determining in advance the sample size needed to apply statistical tests in the future. The hypotheses to be verified are the following:

H_0: there is no trend
H_1: there is a trend

To verify these hypotheses, we use the relation between the power of a Student test, the detected trend level and the desired level of significance (Lettenmaier, 1976):

$$1 - \beta = F_g \ (N_T - Z_{1-\alpha/2}) \qquad (2)$$

where

F_g is the cumulative function of the standardized normal variate;

$Z_{1-\alpha/2}$ is the quantile of the normal distribution for a probability of non exceedence $1-\alpha/2$;

N_T is a number (dimensionless) which takes into account the trend level, the length of the series and is defined according to the kind of the trend considered.

We suppose that the trend, if it happens, will be linear instead of in steps. The expression of N_T for a linear trend is the following (Lettenmaier, 1976):

$$N_T = \frac{Tr}{\sigma_\epsilon} \ \frac{\sqrt{n^*}}{\sqrt{12}} \qquad (3)$$

where

Tr   is the mean level increase during a period of time;

σ_ϵ is the standard deviation of the random component of the series;

n^* is the number of independent samples.

If we fix the power (1 - β) of the test to 0.9, the relation 2 is simplified to:

$$N_T - Z_{1-\alpha/2} = 1.282$$

If we replace N_T by the expression given by equation 3, we then have an equation relating the sample size n^* to a trend level Tr/σ_ϵ and to a significance level α when the power of the test is fixed:

$$n^* = \frac{12 \ (1.282 + Z_{1-\alpha/2})^2}{(Tr/\sigma_\epsilon)^2} \qquad (4)$$

When the sample size is lower than 30, it is better to replace the quantile $Z_{1-\alpha/2}$ of the normal distribution by the quantile $t_{1-\alpha/2;\nu}$ of the Student distribution.

The preceeding equations are valid only for independent samples. In practice, we are often faced with dependent samples in a series; this dependency reduces the information content of the series. We can calculate the information content of a stationary series of n dependent observations by the following relation (Lettenmaier, 1976; Sanders et al., 1987):

$$\frac{1}{n^*} = \frac{1}{n} + \frac{2}{n^2} \sum_{p=1}^{n-1} (n-p)r_p \qquad (5)$$

where   p = interval of time between sucessive observations;
n = total number of observations in the series;
n^* = effective number of observations;
r_p = autocorrelation coefficient for lag p.

The following procedure was then adopted: at first we calculated, for each
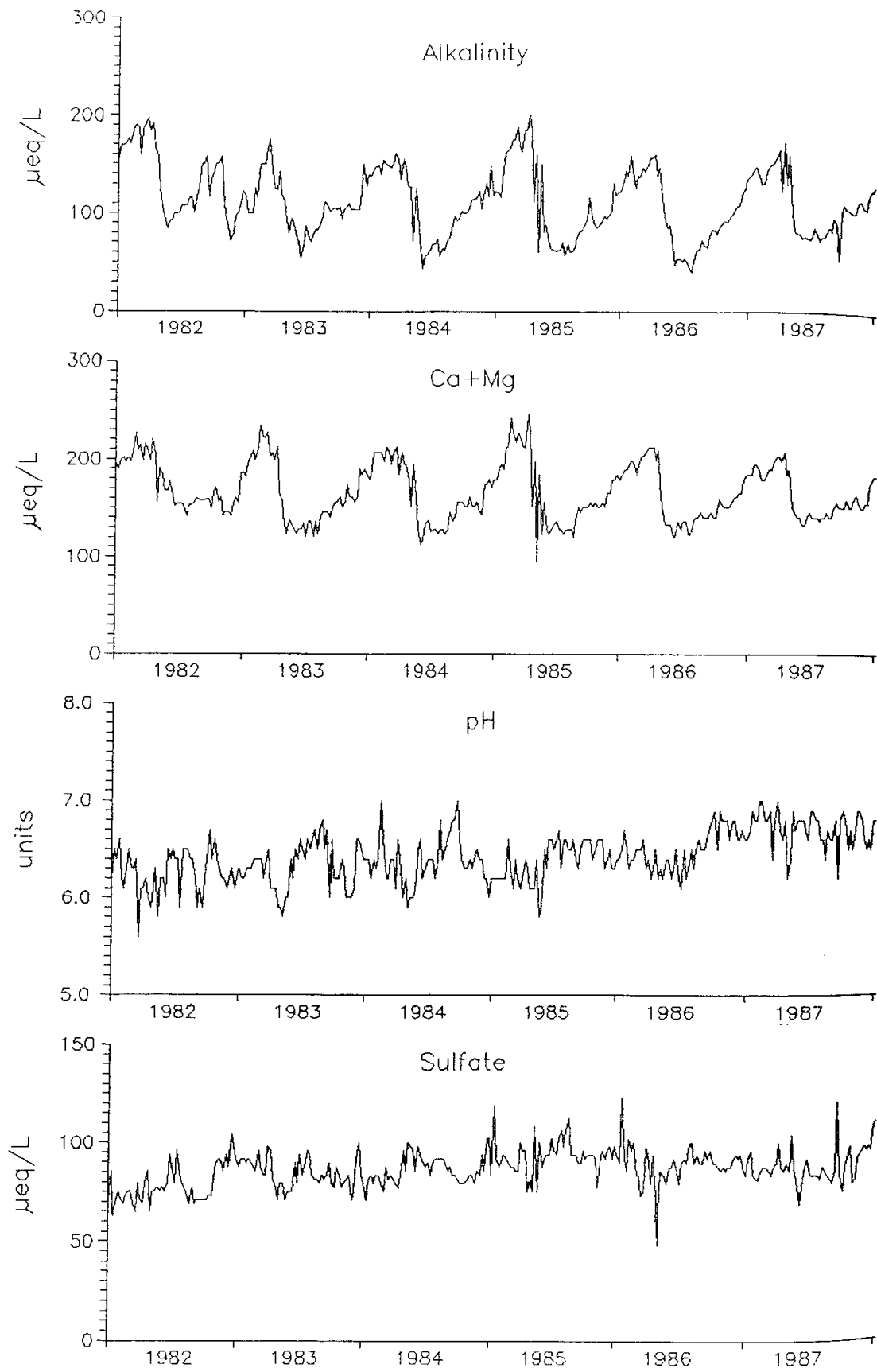
igure 4.   Temporal evolution of alkalinity, Ca + Mg, pH and sulfate on lake Laflamme during the 1982-1987 period.

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physcio-chemical variable, the autocorrelation function on series made stationary; we then calculated n* for different values of n and r_p. To do this, we had had to verify the normality of the distributions. For each of the variables, the normality of the distributions was accepted despite some deviations in the normality for alkalinity and calcium + magnesium (Lachance, 1988).

To obtain stationary series, a seasonal component and a linear trend component have to be subtracted. For the extraction of a seasonal component, we first calculated on each data series (between January 1st 1982 and December 31st 1987), the moving average of the 26 preceding weeks and of the 26 following weeks. This computation was made possible because data were available for the six last months of 1981 and the six first months of 1988. We then obtained the seasonal component by calculating the inter-annual average of the deviations between observed value and moving average for each of the 52 weeks of the year. A deseasonalised series is obtained by subtracting the seasonal component from the initial series.

For each of the deseasonalised series, we then calculated the linear trend by the least squares method. From the random component of the linear regression equation (Lachance, 1988), we have the stationary series on which the autocorrelation function is calculated for the lags 1 to 30 (Figure 5). The standard deviation of the autocorrelation coefficients gives an estimate of the significance level of the latter. We can see that the persistence is significant over a relatively long period of time, notably for alkalinity (13 weeks), sulfate (12 weeks), pH (9 weeks) and calcium + magnesium (7 weeks).

For a given period of time, the effective number n* of observations was calculated according to different numbers n of samples from equation 5. The autocorrelation coefficients r_p used in this equation are the p positive non-zero coefficients calculated from the stationary series. A smoothing of the function (moving average of 5 terms) was

performed in order to correct the coefficients for random fluctuations.

For a weekly sampling frequency (n = 52), the effective number n* of independent observations per year for each of the physico-chemical variables is as follows:

alkalinity	5.1
Ca + Mg	10.0
pH	10.6
sulfate	8.4

This effective number (n*) of observations may be considered as a good approximation of the maximum number (n^*_{max}) of independent observations per year for each of the variables. Indeed we can show (Lachance, 1988) that the increase in the effective independent samples flattens when the number of samples is superior to 40 per year.

The quantity n^*/n^*_{max} may be considered as a measure of the saturation level of information. Therefore, for each variable considered, we can calculate the annual number of samples needed for different informationsaturation levels (Table 2). A compromise may be obtained by calculating the arithmetic average (or weighted average depending on the variables) of annual sampling frequencies of each variable. For a given information saturation level fixed at 80% (reasonable saturation level), an annual sampling frequency of 13 would be needed.

Knowing n* for different sampling frequencies, we can deduce the total sampling period of time to detect trend to standard deviation ratios Tr/σ_ϵ equal to values such as 2.0, 1.5, 1.0 and 0.7 (Table 3). These results show that we cannot hope to detect a trend level Tr/σ_ϵ lower than 1.5 before a reasonable period of approximately 10 years. These results also show that it is not desirable to increase the annual sampling frequency from 13 to 26, as it will not sufficiently reduce the sampling period.

From all the results obtained by the analysis of temporal variability, we can conclude that a monthly sampling frequency is optimal when the high level of persistence in
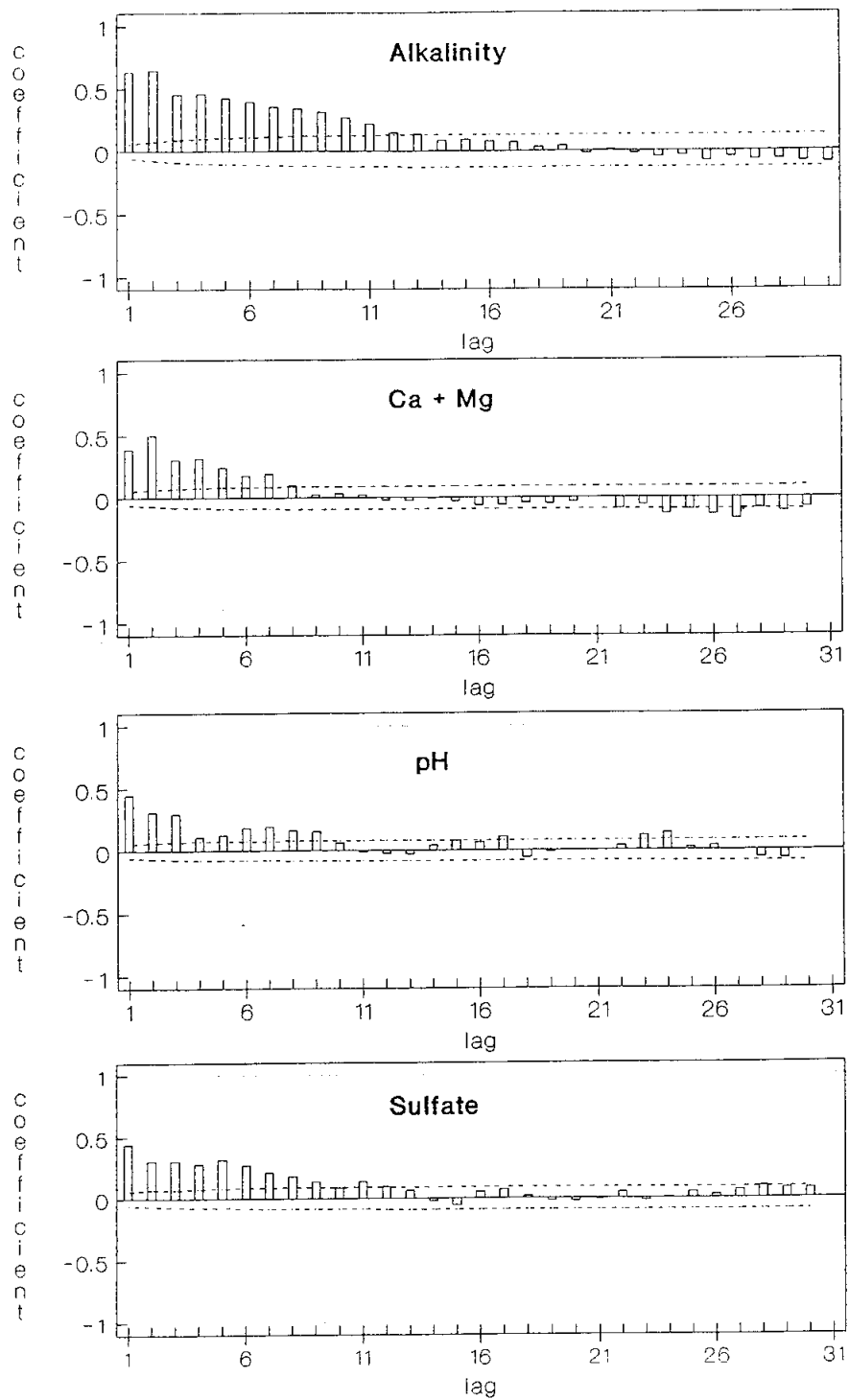
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Figure 5.   Autocorrelation function calculated on stationary series of alkalinity, Ca + Mg, pH and sulfate.

data and the acceptable trend detection level for a 10-year sampling period are taken into account.

SPATIO-TEMPORAL COMPROMISE

We know that to reach one of the objectives, which is the knowledge of spatial variability, we have to allocate a great number of spatial stations sampled at a low frequency. Also, to meet the other objective, which is the knowledge of temporal variability, we had to provide a reduced number of temporal stations sampled at a high frequency. Limited resources generally limit the total number of samples per year to be analysed. To meet both objectives when resources are limited, a sampling plan was drawn up as a result of a spatio-temporal compromise.

The total number of samples N_0 per year fixed by available resources may be expressed as follows:

$$N_0 = K t + L s \qquad (6)$$

where

K = number of temporal stations;
L = number of spatial stations;
t = temporal stations sampling frequency;
s = spatial stations sampling frequency;

If spatial tours are synchronized with visits of temporal stations, the latter can also contribute in providing spatial information. The effective number of spatial stations thus becomes equal to the total number of stations M = K + L.

The total number of samples N_0 per year may be expressed as a function of K and M:

$$N_0 = K (t-s) + M s \qquad (7)$$

If we fix N_0 (say 300), it is thus possible to visualize graphically the relationship between K and M for different values of t (6, 8, 13 or 26) and s (1 or 2) (Figure 6). The graph can

be used as a nomogram that relates the allocation of temporal stations K with the total number of stations M leaving both temporal and spatial sampling frequency fixed.

A quantity π may be defined to express the relative weight of temporal aspects to spatial aspects:

$$\pi = \frac{K t}{M s} \qquad (8)$$

Points corresponding to $\pi = 1$, 2 and 4 have been reported in Figure 6. We can see that this quantity π can be used as a guide when selecting temporal and spatial sampling plan scenarios.

If we fix a reasonable limit for π, say between 1 and 5, and if we choose a frequency of 13 samples per year, we can build 14 spatio-temporal sampling plan scenarios, from a total number of samples $N_0 = 300$, including 9 scenarios with one spatial tour per year (s = 1) and 5 scenarios with s = 2 (Table 4).

To allocate the M spatial stations to the five homogeneous zones, we used the random stratified sampling with optimum allocation method. However, to allocate the K temporal stations, we preferred to use the proportional random allocation method because of the lack of temporal information on the entire region being studied. Because of limited resources, we had to place limits on the minimum number of stations per stratum. For the planned network, we provided a minimum number of temporal stations per stratum: $K_i \geq 2$. In fact, just one station per zone would be insufficient to adequately control the representativity of stations. We also provided a minimum number of stations ($M_i \geq 4$) for the spatial sampling plan.

The selection of two spatial sampling tours considerably reduces the number of spatial stations for a given weight π. If only one spatial tour is carried out, it should then be done during a season with stable hydrological conditions, like winter. A second tour during another season allows us to ascertain the representativity of the sampling season and to make sure that spatial variability does not

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TABLE 3: Total sampling period (in years) needed to detect some trend levels according to different sampling frequencies for a power of the test fixed at 90% and a significance level fixed at 5%.

Tr/σ_ϵ	annual samples	alkalinity	Ca + Mg	pH	sulfate
2.0	6	8.3	6.0	6.3	6.7
	8	7.4	5.2	5.0	5.8
	13	6.8	4.3	4.0	4.7
	26	6.4	3.6	3.3	4.0
1.5	6	14.8	10.7	11.3	12.0
	8	13.2	9.2	9.0	10.4
	13	12.1	7.6	7.1	8.5
	26	11.3	6.3	5.8	7.2
1.0	6	33.4	24.0	25.4	26.9
	8	29.7	20.6	20.2	23.3
	13	27.3	17.0	15.9	19.0
	26	25.4	14.3	13.1	16.2
0.7	6	68.1	49.0	51.8	54.9
	8	60.7	42.1	41.2	47.6
	13	55.7	34.7	32.4	38.8
	26	51.9	29.1	26.7	33.0

Sampling plan scenarios giving the allocation, per stratum, of the number of spatial and temporal stations on the basis of 300 samples per year and a frequency of 13 samples per year.

cenario	s	K	M	π	K_1	K_2	K_3	K_4	K_5	M_1	M_2	M_3	M_4	M_5
1	1	20	60	4.33	2	10	3	3	2	4	20	8	13	15
2	1	19	72	3.43	2	9	3	3	2	4	24	10	16	18
3	1	18	84	2.79	2	9	3	2	2	4	28	12	18	22
4	1	17	96	2.30	2	8	3	2	2	4	33	13	21	25
5	1	16	108	1.93	2	8	2	2	2	4	37	15	24	28
6	1	15	120	1.62	2	7	2	2	2	5	41	17	26	31
7	1	14	132	1.38	2	6	2	2	2	5	45	19	29	34
8	1	13	144	1.17	2	5	2	2	2	6	49	20	32	37
9	1	12	156	1.00	2	4	2	2	2	6	53	22	34	41
10	2	22	29	4.93	2	11	4	3	2	4	9	4	5	7
11	2	20	40	3.25	2	10	3	3	2	4	13	5	8	10
12	2	18	51	2.29	2	9	3	2	2	4	17	6	11	13
13	2	16	62	1.68	2	8	2	2	2	4	21	8	13	16
14	2	14	73	1.25	2	6	2	2	2	4	24	10	16	19

straints for $M_i \geq 4$ and $K_i \geq 2$ for i = 1 to 5;

number of spatial tours per year;

number of temporal stations; K_i (i = 1 to 5) = number per stratum;

total number of stations (spatial and temporal); M_i (i = 1 to 5) = number per stratum;

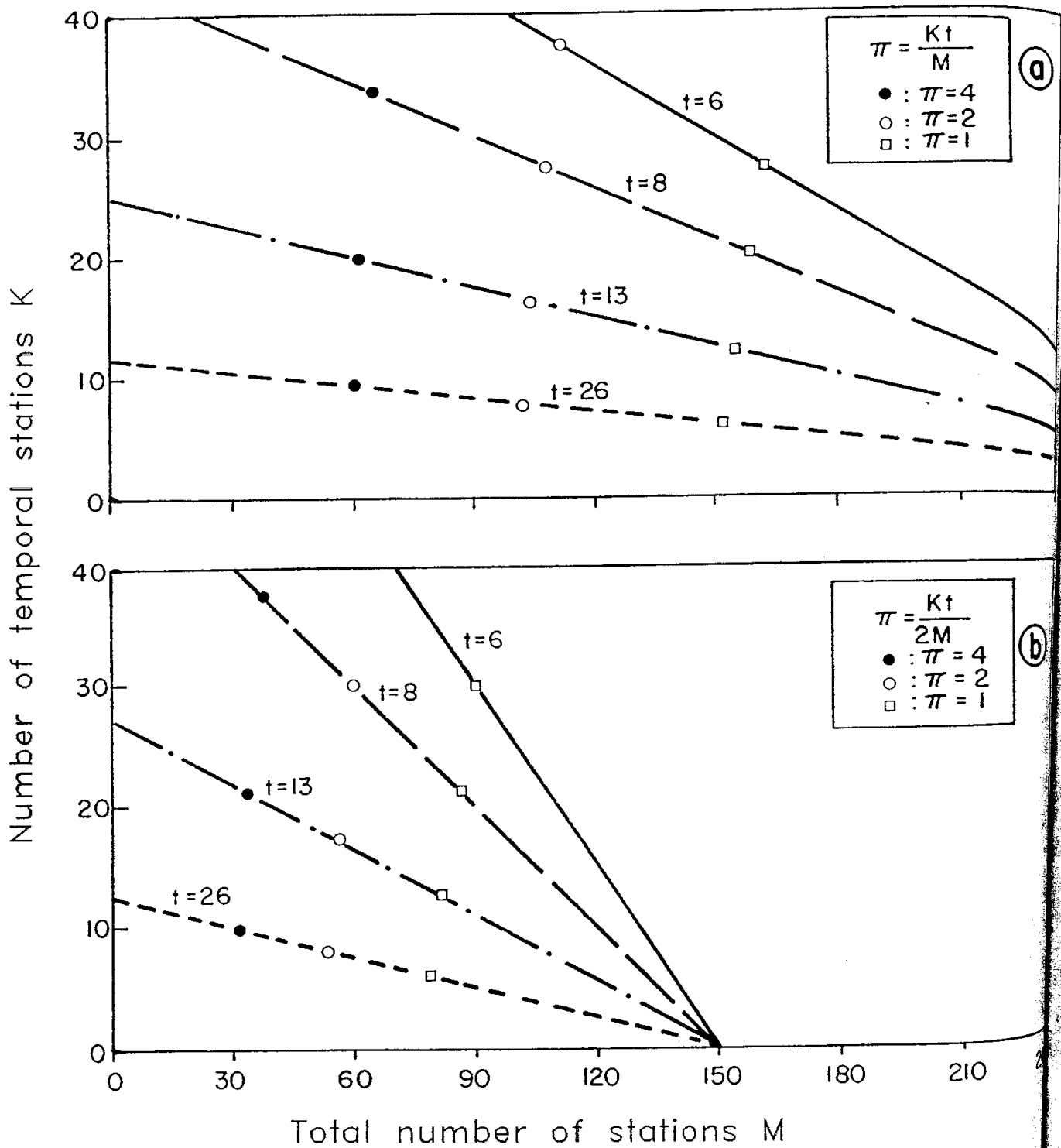relative weight of temporal aspects on spatial aspects.

Figure 6.   Nomogram usable to get the number of temporal stations in relation
            the total number of stations when the sampling frequency is fixed.

result from a seasonal effect. However, in the case where temporal stations are available and allow for this hypothesis to be verified, scenarios with two spatial tours should be eliminated when choosing a spatio-temporal compromise. A choice between different scenarios finally depends on the importance of the temporal or spatial aspects we want to favour. Nevertheless, the final choice depends on the decision of the government agency responsible for establishing the network.

CONCLUSION

We have drawn up a methodology to develop a sampling plan in order to study an environmental problem with temporal and spatial aspects. This methodology was applied here to the design of a trend detection network in the acidification of lakes. A multivariate analysis of spatial information has led to the determination of homogeneous zones that allowed for the application of stratified sampling for spatial aspects. The analysis of the temporal information content of a long series of data, available on a lake of the region, demonstrated that a monthly sampling frequency was essential if a trend is to be detected in a reasonable period (say ten years). Sampling plan scenarios, resulting from a spatio-temporal compromise, were elaborated in order to maximize the acquisition of information, while constraints imposed by available resources were taken into account.

The methodology presented here was developed using two steps. The first step, described in detail by Bobée et al. (1983), has already led to the design and establishment of a sampling network operated by Environment Canada(Haemmerli et al., 1984) to detect trends in the acidification of Québec surface waters. This network, which began operation in 1983, was initially composed of 35 stations used to study spatial aspects, 10 of which were sampled every two months for the study of temporal aspects. As we can see, this sampling plan is somewhat different from the sampling scenarios proposed in this study, but was developed with a similar procedure using data available at that time.

The methodology described here for the design of such a network can be used for wider regions such as Eastern Canada, and can also be applied to the study of other environmental problems.

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REGIONAL SURFACE WATER QUALITY CHARACTERISTICS OF NEBRASKA

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ABSTRACT

The ability to identify regional differences in water quality characteristics provides resource managers with an important tool. This information can be used to develop cost-effective monitoring networks, set regional water quality standards and identify areas of non-conformity where remedial actions may be needed.

Water quality data from 69 ambient monitoring stations in Nebraska were evaluated for regional patterns using principal component analysis and cluster analysis. Principal component analysis reduced the data set of nine parameters to three components: ionic strength, runoff, and nitrogen. These three principal components explained 80% of the variation in the original data set. Clustering of the median values of the principal components resulted in good spatial correspondence between water quality characteristics as measured by the principal components and the Soil Conservation Service's Major Land Resource Areas.

Management implications of these defined regional characteristics are significant. The results of the principal component analysis suggest that parameter coverage, and hence cost, can be reduced without loss of the information content at the monitoring locations. Based on cluster analysis, decisions can be logically made about the necessary extent of the monitoring network and about the water pollution control activities needed in areas with atypical water quality characteristics.

INTRODUCTION

Information on the spatial variation of water quality characteristics can be a valuable water quality assessment tool for water quality managers. The ability to identify regional differences and similarities in water quality characteristics provides decision makers with several program development opportunities. For instance, the information gained from a knowledge of regional patterns can provide the ability to develop region-specific water quality criteria, to target non-point source pollution controls, to design and implement cost effective monitoring strategies, and to more accurately predict the benefits of projects based on the historic results from similar regions.

The concept of water quality regionalization can be logically induced from the observed spatial variation of factors which influence water quality. Precipitation in a watershed will integrate the natural effects of soil, topography, climatic conditions, vegetation, and geological factors with the man-induced effects of point source discharges, agricultural development and use, and infrastructure as it traverses the watershed. Thus, the streams draining regions which are similar with respect to these factors will tend to be similar to each other with respect to water quality characteristics and, conversely, dissimilar to the streams draining regions that are different with respect to these factors.

There are two different approaches to the assessment of regional water quality patterns.

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The first approach applies any of the numerous data aggregation techniques (such as cluster analysis, analysis of variance, discriminate analysis, or multiple regression analysis) to site specific data. This method allows the data to define regions without prior definition of regional patterns. The second approach selects a regional classification system and then uses existing or specifically collected data to test the hypothesis that the data associated with a given region are in fact different from those of another region.

The first of these regionalization methods has been utilized to assess regional patterns of both fish community assemblages and water quality characteristics. Pflieger (1971) and Pflieger et. al. (1981) used this approach to describe the distribution of fish in Missouri; Legendre and Legendre (1984) used it to explain postglacial fish distribution in Quebec; and Hawker et. al. (1987) used it to define fish ecoregions in Kansas. These techniques have been used to define regional water quality characteristics by numerous researchers. Steele and Jennings (1972) used them in Texas; Steele et. al. (1987) used them in a portion of West Germany; and Herskary et. al. (1987) used them for the trophic classification of lakes in Minnesota.

The second approach to regionalization has utilized a variety of land classification systems. Smart and others (1981) utilized physiographic provinces of Missouri to regionally assess water quality. In Iowa, Paragamian (1986) reported regional differences in the standing stocks of various fishes based on the physiographic region of collection. More recently, a great deal of interest has been directed towards the correspondence of water quality characteristics and fish communities to Omernik's (1987) national aquatic ecoregions. Aquatic ecoregions have been used as the basis for regionalization in Ohio by Larsen et. al. (1986), in Oregon by Hughes et. al. (1987), and in Arkansas by Rohm et. al. (1987).

The Soil Conservation Service's (1981) Land Resource Area (LRA) categorization includes many of the same factors as Omernik's Aquatic Ecoregions. However, LRA divisions generally cover a smaller area and are primarily based on agriculturally related factors. The greater possibility for resolution of real differences in water quality characteristics and the preponderance of agricultural activities in the midwest suggest that LRAs may provide a basic tool for the development of regional water quality characteristics.

The objectives of this study were to:

1. Determine if regional water quality differences exist in Nebraska,

2. determine if a correspondence exists between water quality characteristics and the Soil Conservation Service Land Resource Areas, and

3. identify management implications of defining regional water quality characteristics.

METHODS
Data Selection

An assessment of regional patterns of surface water quality in Nebraska was conducted utilizing data that had been collected by the Nebraska Department of Environmental Control and the Water Resource Division of the U.S. Geological Survey and stored in EPA's STORET Water Quality File.

These two agencies collect water samples for a variety of reasons including long term trend monitoring, ambient water quality assessments, and project planning or evaluation. However, only two restrictions were placed on the data retrieved for the assessment. First, the data must have been collected after January 1, 1981. This restriction was imposed to ensure that the data used had been collected and analyzed in accordance with the Nebraska Department of Environmental Control's Quality Control/ Quality Assurance Program Plan. Second, the data must have been collected from stations where there were at least four records in a twelve month period, and adequate data (i.e. not excessive missing values) for the parameter monitored.

These criteria resulted in the selection of 69 stations and nine parameters for subsequent analysis. The nine parameters were: Specific conductance, total dissolved calcium, total dissolved magnesium, total dissolved sodium, total organic carbon, total phosphorus, suspended solids, total ammonia, and total nitrate and nitrite-nitrogen. The stations selected are shown on Figure 1.

Data Analysis

Cluster analysis was the primary method of identifying the correspondence between water quality characteristics and Land Resource Areas. This procedure was conducted following several data purging and reduction steps. All statistical procedures were performed utilizing SAS (1986).

Initial analyses revealed that none of the nine variables were normally distributed. In order to normalize the data set, all variables were subjected to a logarithmic transformation and then tested for normal distribution. This transformation successfully normalized the distributions of all the variables of interest.

Following transformation, the normalized data set was subjected to Principal Component Analysis with varimax rotation utilizing the SAS FACTOR PROCEDURE. Only those principal components with eigenvalues greater than or equal to one were retained, since principal components with eigenvalues of less than one provide no more information that a randomly generated variable (Legendre and Legendre, 1983). At each station, the median values of a significant principal components (e.g. those with eigenvalues greater than or equal to 1) were computed to provide the least biased estimate of the central tendency for the station.

Cluster analysis was performed on the median values of the principal components using the FASTCLUS procedure. Since there are no established criteria for determining the number of clusters in a data set (Romesburg, 1984), the number chosen was thirteen, which is the number of Land Resource Areas in Nebraska (Figure 2). This number criteria was chosen in order to obtain maximum

resolution of spatial differences which could be attributed to Land Resource Areas.

RESULTS

Principal component analysis with varimax rotation provided a useful mechanism for evaluating water quality characteristics. This procedure was able to reduce the nine original variables to three significant components which were able to explain approximately 80 percent of the variance in the original data set. The principal components, the variables associated with each, and the variable loadings are presented in Table 1.

Principal component 1, which consists of conductivity, dissolved calcium, dissolved magnesium and dissolved sodium, represents the ionic strength characteristics of surface water. This principal component explained 42 percent of the variation in the data. The composition of this component is consistent with geological and land use characteristics of Nebraska. The availability of both surface water and ground water for irrigation and subsequent irrigation return flows as well as the intimate relationship of surface water and ground water in large areas of Nebraska primarily account for this component.

Principal component 2, which is comprised of suspended solids, total organic carbon and total phosphorus, represents the non-point source or errosional characteristics of the watersheds. This run off component explains approximately 27 percent of the data set variance.

Principal component 3, the final significant component, consists of ammonia and nitrates. This component explained 11 percent of the variance. Unlike components 1 and 2, the water quality processes which this component defines are not obvious. The loading of ammonia may represent point source functions, while that of nitrates may represent groundwater characteristics or the combination may represent nitrogen sources associated with agriculture. This component may represent any or all of these processes, depending on the location of interest, and thus is best
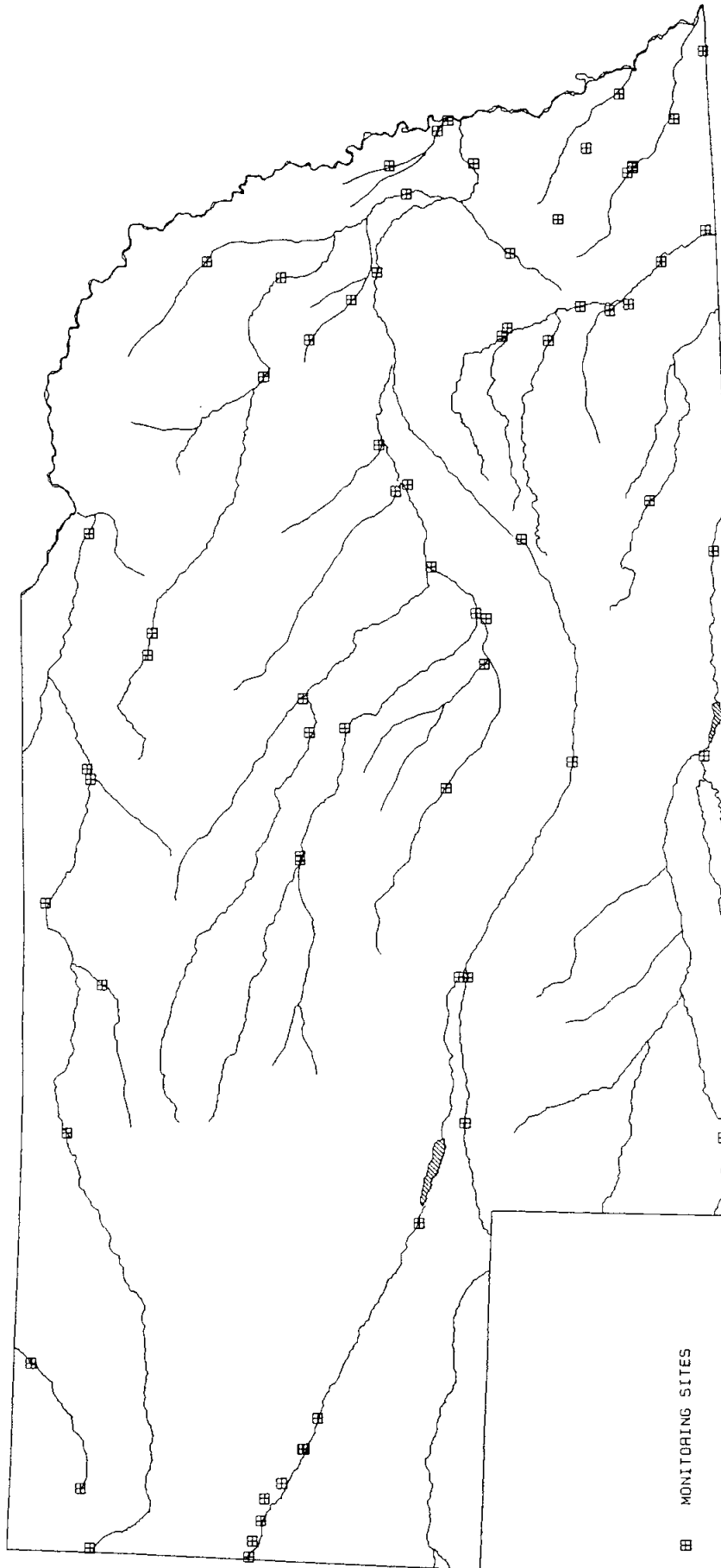
165

FIGURE 1

MONITORING SITES

⊞ MONITORING SITES

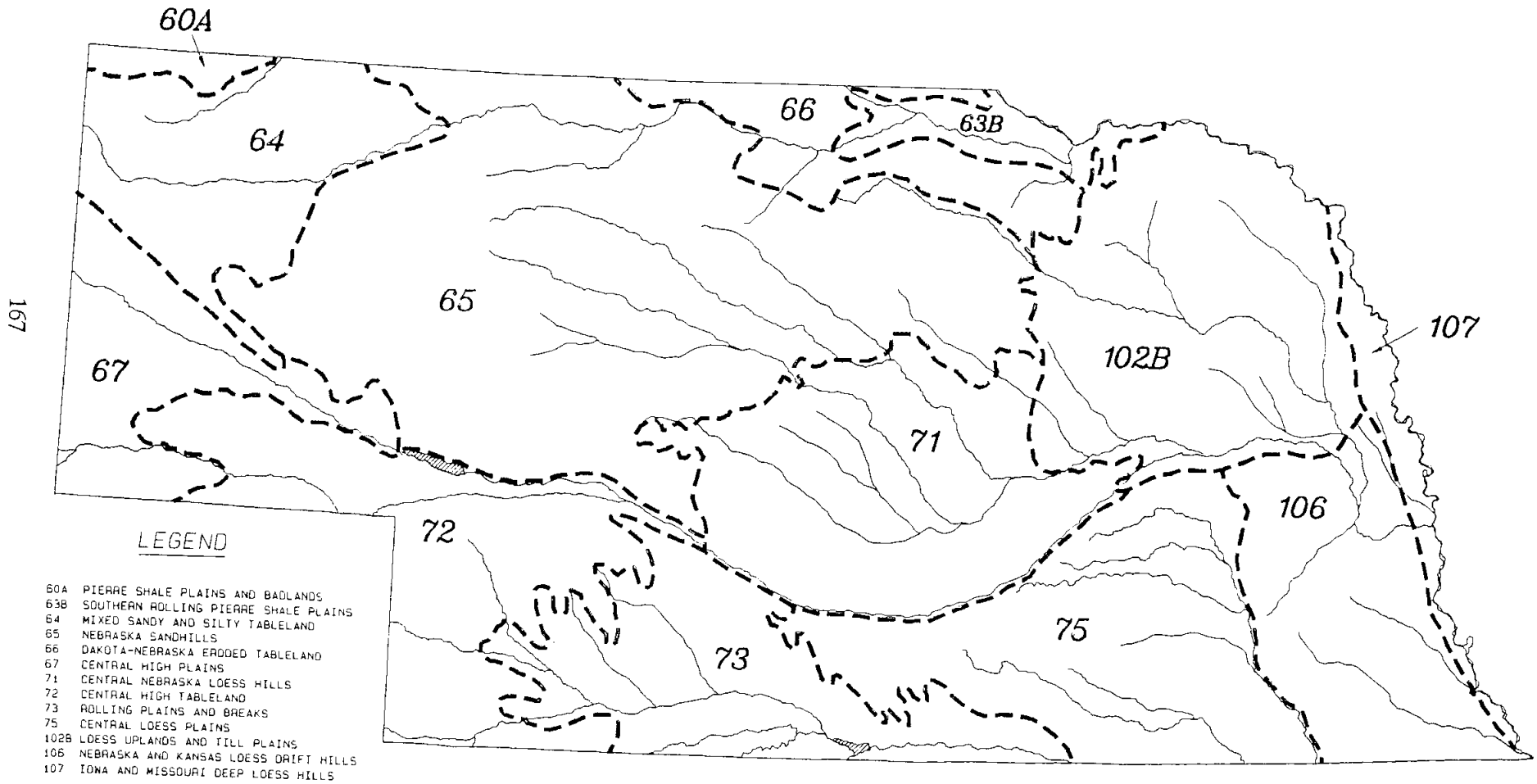## FIGURE 2
MAJOR LAND RESOURCE AREAS

LEGEND

60A PIERRE SHALE PLAINS AND BADLANDS
63B SOUTHERN ROLLING PIERRE SHALE PLAINS
64   MIXED SANDY AND SILTY TABLELAND
65   NEBRASKA SANDHILLS
66   DAKOTA-NEBRASKA ERODED TABLELAND
67   CENTRAL HIGH PLAINS
71   CENTRAL NEBRASKA LOESS HILLS
72   CENTRAL HIGH TABLELAND
73   ROLLING PLAINS AND BREAKS
75   CENTRAL LOESS PLAINS
102B LOESS UPLANDS AND TILL PLAINS
106 NEBRASKA AND KANSAS LOESS DRIFT HILLS
107 IOWA AND MISSOURI DEEP LOESS HILLS

TABLE 1

RESULTS OF PRINCIPAL COMPONENT
ANALYSIS OF NINE WATER QUALITY
VARIABLES MEASURED AT 69 SITES IN NEBRASKA

	Component 1	Component 2	Component 3	
Conductivity	0.975			
Magnesium	0.943			
Sodium	0.902			
Calcium	0.853			
Suspended Solids		0.873		
Total Organic Carbon		0.873		
Total Phosphorus		0.748		
Ammonia			0.858	
Nitrates			0.717	
Percent Variance Explained	.42	.27	.11	TOTAL .80

referenced as simply a nitrogen component. Regionalization was obtained by clustering of the median values of principal components 1, 2, and 3 for each station. A comparison of the cluster membership of each station with the Soil Conservation Service Land Resource Areas (LRA's) demonstrated good correspondence between the clusters and the LRA's. This correspondence is shown in Figure 3.

In a few portions of the state, the correspondence between clusters and LRA's was not as well defined as in other regions. Factors which may contribute to the low level of correspondence are: the inflow of water from an upstream LRA which "masks" the characteristics of the downstream waters, the imprecise resolution of landscape differences by either the SCS classification system or the data analysis techniques, or anthropogenic contribution such as that from wastewater treatment facilities or irrigation returns.

The first factor, (the influence of upstream water) is apparent in the area of transition from LRA 65 to LRA 71. As can be seen in Figure 3, some stations are within LRA 71 but continue to exhibit a cluster membership which is characteristic of the upstream LRA, LRA 65. The impact of LRA 65 continues downstream until a significant level of "dilution" has occurred.

At the station labeled A (Figure 4), approximately 97 percent of the upstream drainage area and 94 percent of the mean stream flow is associated with the upstream LRA. At station B, LRA 65 still accounts for 85 percent of the drainage area and 82 percent of the mean flow. Both of these stations continue to display the characteristics of cluster 6, the cluster associated with LRA 65. At station C the percent contribution of LRA 65 to the drainage area is reduced to 60 percent and its contribution to the mean flow is reduced to 55 percent. At these levels of "dilution", station C exhibits membership in LRA 71's cluster, which is cluster 13.

With respect to the second factor, LRA 66 and LRA 65 best illustrate the imprecise nature of the classification system. As can be seen in Figure 5, the stations within cluster membership as 2's do not correspond in membership to the remainder of LRA 65. This difference and the proximity of LRA 66 suggest that the LRA boundary may be inappropriately drawn for the purposes of this study, and would be better represented by moving the boundary further south. Clusters at the interface of LRA's 60A and 64 also results in poor resolution which can be attributed to boundary locations (Figure 3).

While the cause of an anthropogenic disturbance may not be readily determined from the graphical presentation of cluster membership and LRAs, locations where anthropogenic factors play a role in determining water quality characteristics could be identified. Two such areas are shown on Figure 6. In the area identified as A, the presence of cluster 12, (the only station with that membership) signals the likelihood of an anthropogenic contribution. Additional evaluation of conditions in that area indicate that irrigation return flows appear to be the cause of this cluster membership.

In the area identified as B the presence of cluster 3 strongly suggests an anthropogenic cause. As with cluster 12 in area A, additional evaluation identified the cause. The station which produced this cluster is located immediately downstream of several point source discharges, (a municipal wastewater treatment plant and two nitrogen fertilizer production facilities).

Since principal component analysis had successfully reduced the number of variables, defined major water quality processes, and explained the majority of the variance in the original data set and cluster analysis of the principal components had indicated good spatial correspondence between clusters and LRA's, an analytical method which combined these techniques would likely provide useful water quality information. The technique chosen was to ordinate, by LRA, the three principal components. The results of this technique are shown in Figure 7.

From a management standpoint, Figure 7 provides significant water quality information and can provide the basis for several decisions such as the refinement of existing monitoring programs, the establishment of realistic water

FIGURE 3
CORRESPONDENCE OF PRINCIPAL COMPONENT CLUSTERS
AND LAND RESOURCE AREAS
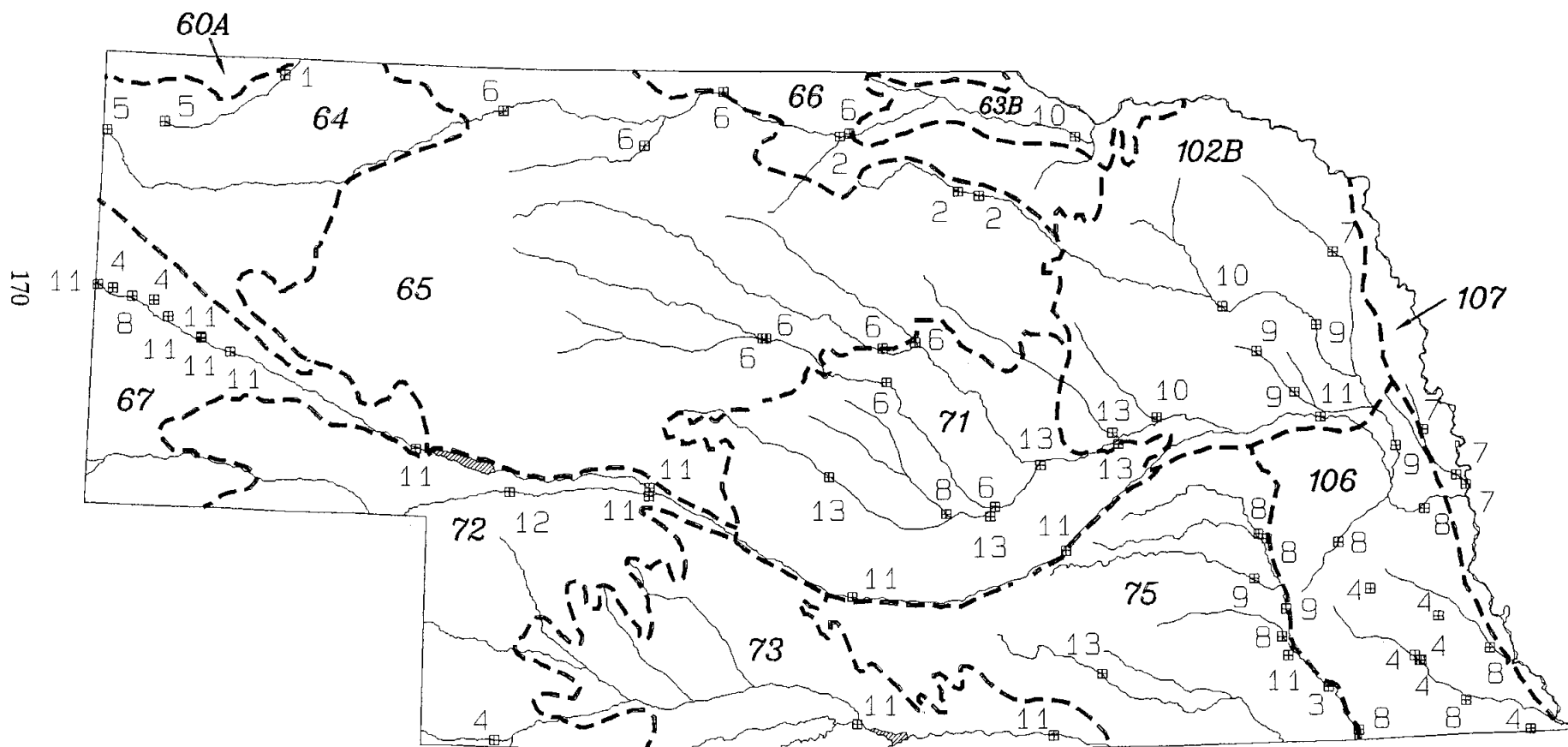
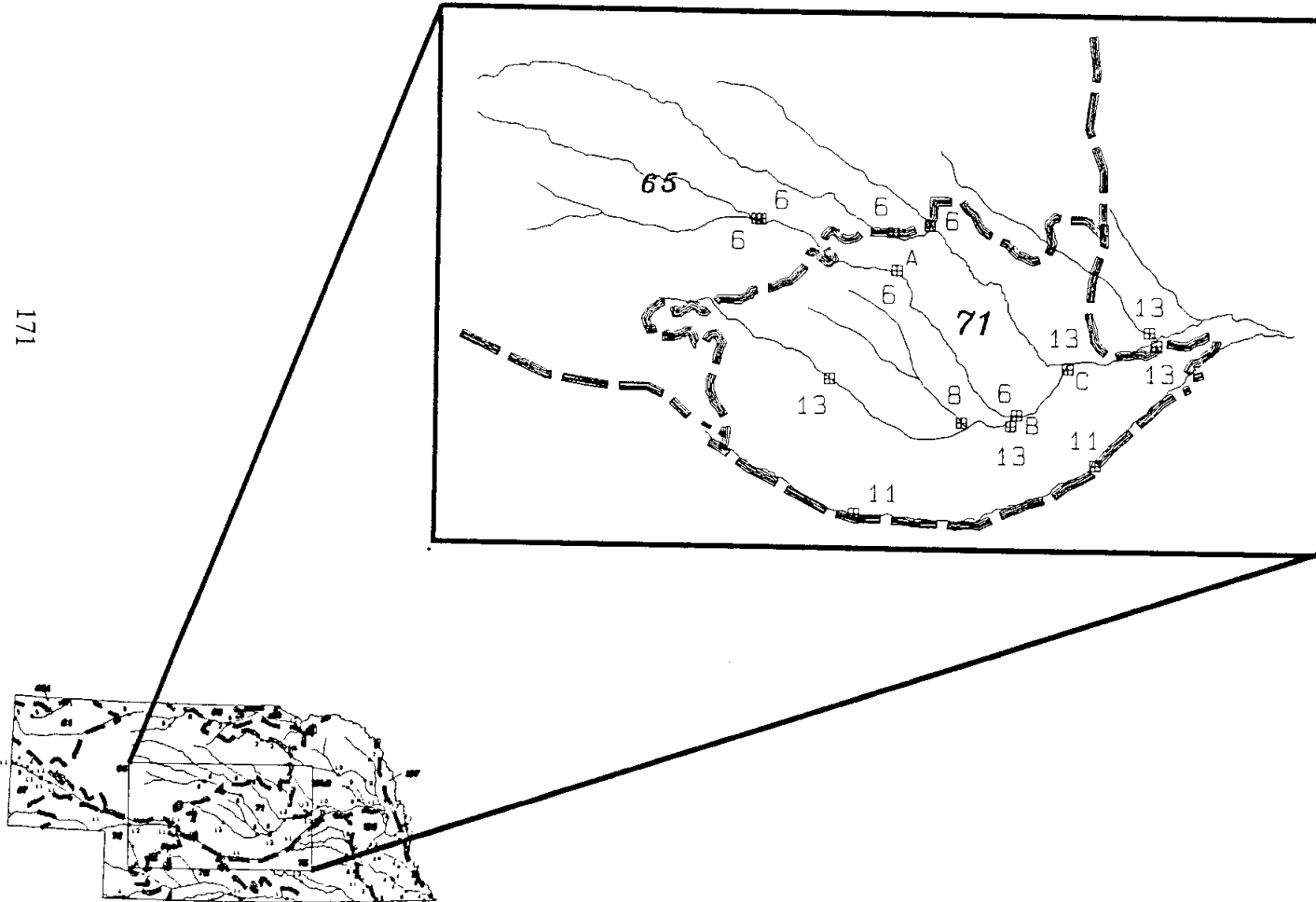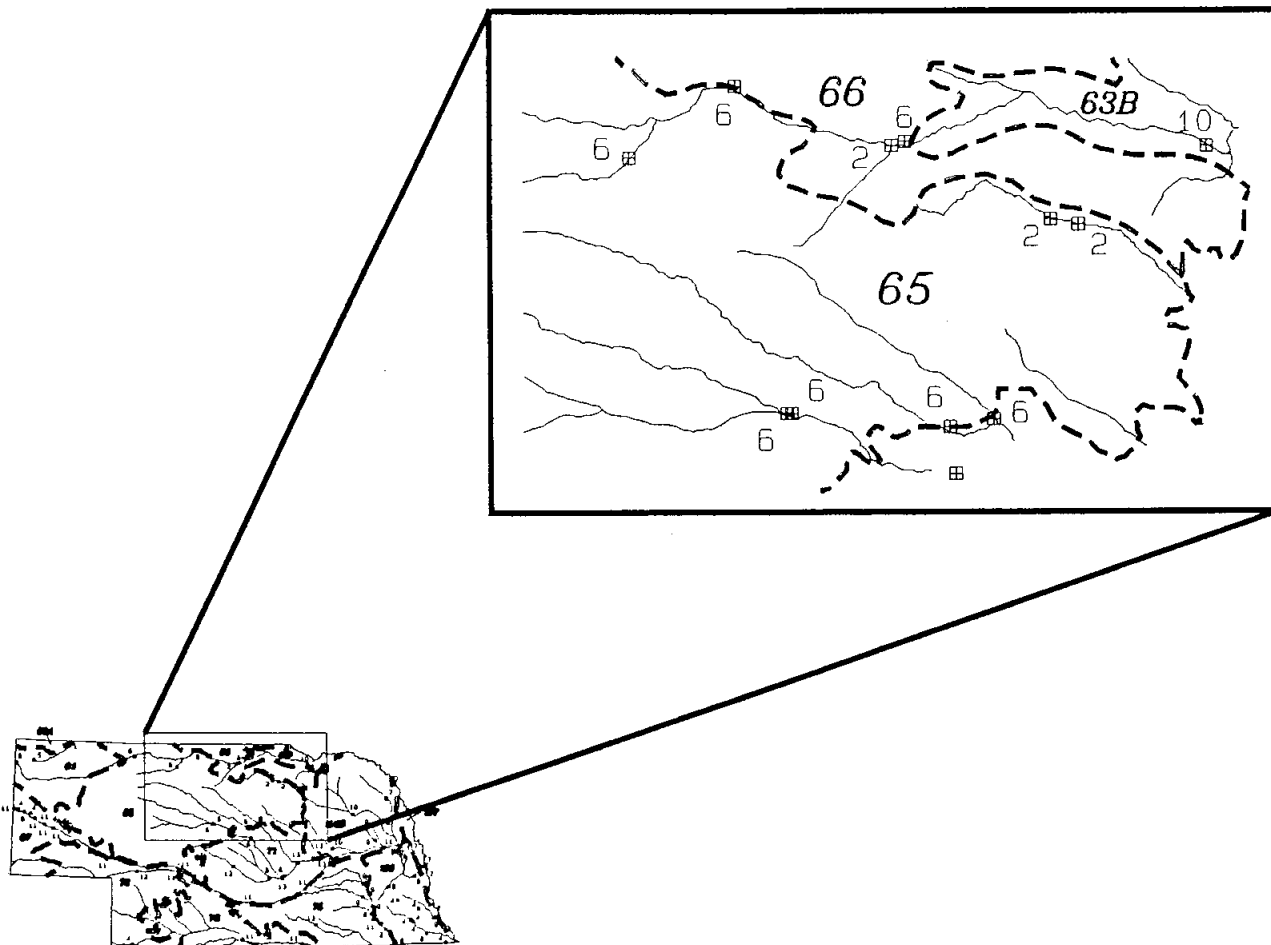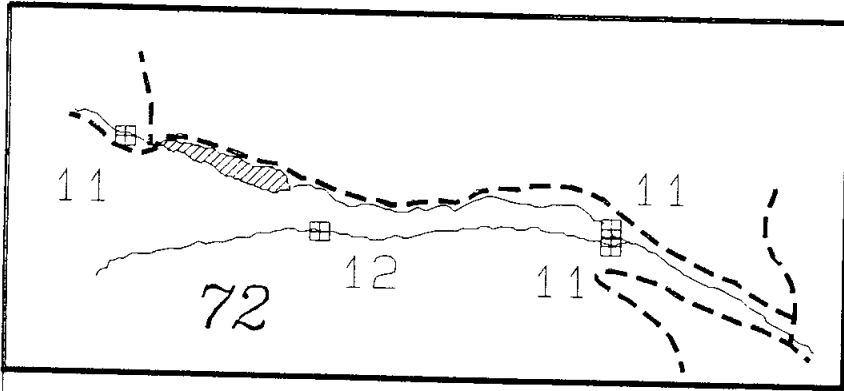# INFLUENCE OF INFLOW FROM AN UPSTREAM LAND RESOURCE AREA

FIGURE 5
EXAMPLE OF CLASSIFICATION OR ANALYSIS
ERROR ON REGIONALIZATION

FIGURE 7
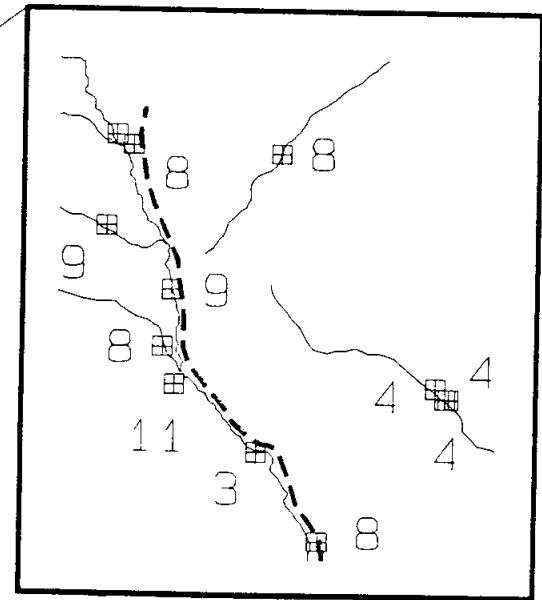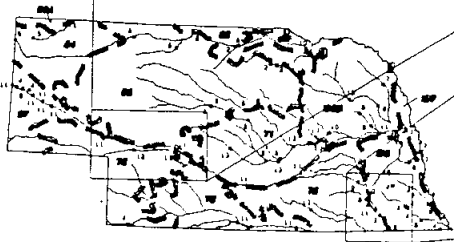## ORDINATION OF PRINCIPAL COMPONENTS BY LAND RESOURCE AREA

quality criteria and the identification of environmental pertutbution.

Within the realm of network design, LRAs which contain numerous monitoring stations and are very homogenous with respect to the principal components, (such as LRAs 64, 65, 67, 73 and 107), would be logical candidates for the critical reviews of the needs at each station. Given the constraints of the intended use of the data collected at each station, it would appear that the number of stations could safely be reduced without information loss.

In LRAs where the principal components are very heterogeneous (LRAs 75, 102b and 106), heterogeneity may be a signal that insufficient data are being collected to adequately assess water quality.

The management decision which could logically be reached from the evaluation of these patterns may be to maintain the present level of resource investment in monitoring but to relocate the investment by reassigning stations from the homogenous LRAs to the heterogeneous LRAs.

In several of the LRAs, especially LRAs 65, 67, and 107, the distribution of the principal components was homogenous within the LRAs but very heterogeneous between LRAs. These clear divisions lend themselves to the establishment of region specific water quality standards and attainable criteria.

Using LRAs 65, 67, and 107 as examples, it can be seen that there are distinct differences in principal component 3 (the nitrogen component) between these LRA's. The use of instream concentrations of ammonia and/or nitrogen in LRA 65 as the benchmark or attainable water quality goal for the entire state would require a significant resource investment in pollution controls with only limited likelihood of achieving the benchmark. On the other hand, selection of the levels attainable in LRA 107 as the state-wide goal would allow water quality in LRAs 65 and 67 to be degraded without consequence.

The most precise and equitable method of establishing criteria would be apparently based on regionalization. For the LRAs which are homogenous, the selection of the attainable criteria is straight forward. For the more heterogeneous LRAs, attainable water quality criteria can best be defined using the regional reference site concept as proposed by Hughes et. al. (1986).

CONCLUSIONS

The analyses of surface water quality data from Nebraska by the multivariate analysis technique of principal component analyses and cluster analysis reveal that spatial patterns exist in water quality. These spatial patterns correspond very well to Soil Conservation Service Land Resource Areas.

Ordination of the principal components by Land Resource Area provides a very effective method of summarizing the analytical results so that management decision on the extent of monitoring systems and attainable water quality criteria can be developed.

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Ensuring Adequacy of Data Records
for Statistical Analysis

QUALITY CONTROL IN THE ANALYSIS OF TRACEL METALS IN GROUNDWATER: A CASE STUDY FROM LAKE TYRRELL REGION, VICTORIA, AUSTRALIA

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ABSTRACT

The need for the collection and analysis and large number of samples distributed over large areas is critical to the evaluation of both local and regional groundwater quality. However, with the need for the collection of many samples in a short time period comes the potential problem of sample contamination during sample collection, handling, storage and analysis. This is particularly true in the case of such environmentally important elements like trace metals which occur naturally at trace to ultra trace levels in most natural waters. If precise and accurate data are to be obtained, great concern and care must be exercised in all aspects of sample manipulation.

We present data for the trace metals, Pb, Cu and Zn, from a series of samples from a saline, low pH groundwater system in NW Victoria, Australia. Along with the groundwater data we evaluate the need for care in obtaining anoxic samples in order to minimize oxidation effects as well as develop a method for determining field blanks. In addition, we discuss the effect on data quality of: 1) the choice of filtration apparatus; 2) type of sample containers; 3)sample container preparation. Knowledge of potential pitfalls in these areas are imperative if representative trace metal data are to be obtained.

INTRODUCTION

Two important questions posed by this symposium are: what is the quality of water? and what do we get for the money we spend on monitoring? The answers to both of these questions are directly dependent on one important consideration, that is, the quality of the data obtained in the monitoring programs. It is obvious that if the quality of the data is poor then the quality of the water is unknown and our money has been ill spent. Therefore, quality control by individual investigators as well as the ability to scrutinize the published literature to determine the "quality" of water quality data are utmost importance to our understanding of the role of both natural processes and anthropogenic activities in controlling water quality. This is particularly true in the case of environmentally important elements like trace metals. Many trace metals are potentially toxic at moderate to trace levels of concentrations and they exist naturally at trace to ultra trace

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levels in most natural waters. In addition because of the potential for changing their in-situ concentrations during sample collection, storage and analyses, the analysis of trace metal samples in natural waters is fraught with difficulty. Contamination and faulty analytical procedures are the most obvious problems in measuring trace metals accurately and precisely in natural waters but other considerations, like changes in redox conditions prior to sample fixation, can also be important.

In this paper we present data from a series of saline groundwater samples from NW Victoria, Australia. We discuss our data for Fe, Pb, Cu and Zn in light of the quality control evaluation during the collecting, handling and analyzing of these samples. We acknowledge that much has been written about the individual aspects in this study. In addition, we suggest an approach to trace metal monitoring whereby quality control can be maintained.

Field Area and Research Rationale

Lake Tyrrell is a large (26 x 7 km) salt-playa lake location in NW Victoria Australia (Fig. 1). The lake became dry approximately 32,000 BP, but is covered with 10's of cm of water for approximately 3 months of the year (Bowler, 1986). The lake contains thin beds (3 m of clay silt and sand covered by an ephemeral halite/gypsum crust (30-60 km). It is underlain by a large aquifer system formed by the Parilla Sand, which is enclosed by the Blanchtown Clay and Geera Clay in the Lake Tyrrell region (Macumber, 1983). The Parilla Sand Aquifer is an uncemented, felspathic-quartz sand, well known in Australia for its heavy mineral content. Decaying algal mats occur locally on the lake floor.

Evaporation greatly exceeds precipitation and recharge to the basin from surface water rarely occurs (Macumber, 1983). Thus, groundwaters in the basin are recharged by direct infiltration of precipitation and by inflow through the regional Parilla Sand aquifer. The groundwater can be characterized by salinity and location into 3 major types:

1. Water from the Parilla Sand Aquifer have salinities similar to seawater (4%) and specific gravity of 1.05 g/km^3. The waters are oxic, have pH's less than 4, and enter the Lake Tyrrell as seeps along the western shore. These waters flow onto the lake surface on the western side of the lake in "spring" or discharge zones.

2. Brines which saturate the Parilla Sand below Lake Tyrrell are formed by evaporitic concentrations and reflux of groundwater. This water is denser (1.16 g/cm^3) and more saline (25%) than regional groundwater. The waters are anoxic with near neutral pH's.

3. Brines beneath two small lakes east of Lake Tyrrell, Lakes Wahpool and Timboram are also formed by evapo-concentration of regional water, but have salinities about half that of the Lake Tyrrell reflux brine (12%) and specific gravities of 1.09 g/cm^3. These waters are anoxic with near neutral pH's and enter the lake as seeps along the eastern shore.

Processes associated with the origin and chemical evolution of hypersaline systems have been demonstrated to be of great geological, geochemical and practical significance. For example, over the past 15 years many models have been proposed to explain how metals accumulate in low temperature, low pressure systems to form ore deposits. In many cases, these models are linked to geological processes in hypersaline environments (e.g., sabkhas, closed basins) (Renfro, 1974; Eugster, 1986). Yet, the role of hypersaline environments in the formation of low-temperature ore deposits is unclear, because modern day analogs of ore forming systems are not well known and the behavior of trace metals in hypersaline systems is not well documented.

Our goal at Lake Tyrrell was to identify the hydrological, mineralogical, biogeochemical, and sedimentological processes occurring during metal accumulation
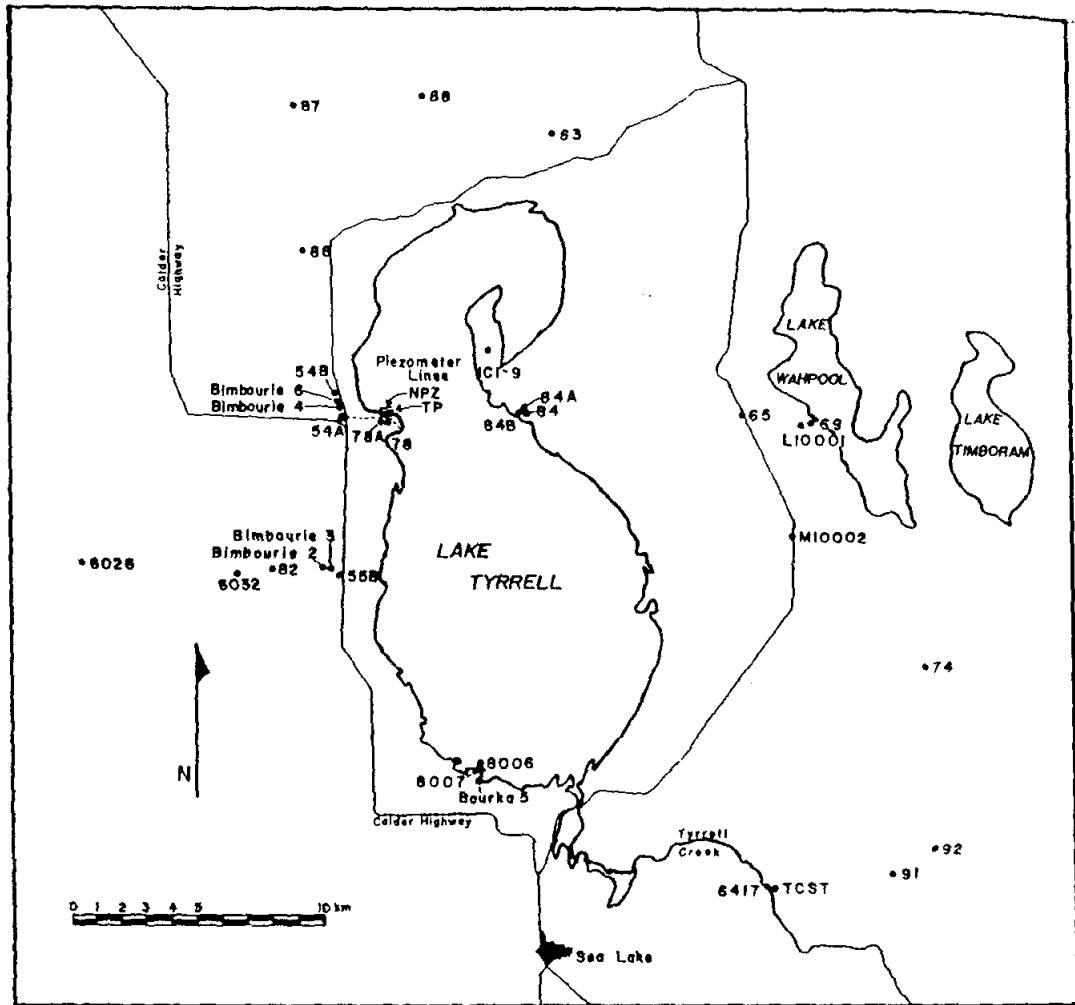
Figure 1.

in or near the lake so that the role of hypersaline environments in the formation of low temperature ore deposits could be assessed. The framework for this research was to consider the source of metals to the system, the source of sulfide (or processes tending to enrich the sediment in metals) and the mechanisms of getting the sulfide and metals to mix (or the description of the hydrology of the system). The detailed results of the geochemical and sedimentological studies will not be presented here. In order to establish whether or not the Lake Tyrrell sediments are a "sink" for trace metals, a detailed sampling survey of the regional groundwater (RGW) as well as the fore-mentioned reflux brine (RB) was undertaken. Because the characteristics of the RGW hydrology are well known (Macumber, 1983), the RGW could be sampled along a flow path toward the lake and finally onto the lake's surface in the "spring" zone areas. From this information, a sample box model could be developed to estimate metal removal from the RGW into the lake sediments. Accurate and precise determinations of the metal concentrations of all the Lake Tyrrell waters was needed in order to accomplish this.

Because this is essentially a "methods" paper, we will present our methodology in detail. This section will be sub-divided into the following categories: 1) cleaning, 2) sample collection, 3) sample storage, 4)sample analyses and 5) blank determinations. The neglect of any of these categories during monitoring of trace metal water quality can lead to erroneous results. Much can be learned from the marine science community in this regard. Although trace metal data from various parts of the world ocean were collected and analyzed prior to 1975, little of it was accurate. This was due primarily to contamination during sampling and analysis. The work of Patterson and the convening of funding agency sponsored inter-laboratory intercalibration exercises (Brewer et al., 1974; Bewers et al., 1976; Patterson and Settle, 1976) made it painfully clear that the risk of sample contamination for Pb and probably other trace metals was indeed real. Since 1975, marine chemists have developed a more accurate picture of trace metal distribution in the oceans. This did not come about without

close attention to detail to eliminating contamination risks. Non-marine water chemists have also recognized the inherent problems in collecting and analyzing natural water samples for trace metals. (e.g.. Hume, 1973; Batley and Gardner, 1977; Subramanian et al., 1978; Truitt and Weber, 1979; Owens et al., 1980; Rpt. by the German Chemists Assoc., 1981). However, when one reads the terrestrial water literature one learns that many investigators fail to provide enough detail in the categories listed above to establish the quality of their trace metal measurements.

Often water monitoring programs are intent on producing the largest amount of data in the shortest amount of time. This may be done in ignorance of the trade-off between haste and strict quality control. A lack of detail to potential contamination and/or analytical problems may produce data sets that are virtually meaningless. Therefore, all individuals involved in water monitoring of trace metals must develop an awareness of these potential pitfalls.

METHODS

Cleaning Procedures

Patterson and Settle (1976) have emphasized the need for proper sample container cleaning if ultra trace analysis of Pb is to be undertaken. This has also been made clear for other metals like as Cu, Cd, Zn and Ni (Bruland et al., 1979) and for sample collection apparatus (Fitzgerald and Lyons, 1975; Spencer et al., 1982; Simmons, 1987). Trace metal impurities in materials that come into contact with samples can easily invalidate the data. Carefully cleaned polyethylene and/or teflon bottles have been the containers of choice in previous trace metal storage studies (Batley and Gardner, 1977; Subramanian et al., 1978). In our Lake Tyrrell study we utilized the following materials: for sample collection of groundwaters, a teflon bailer, for sample filtration, a teflon filtering unit and for sample storage, either Nalgene^{TM} linear polyethylene or polypropylene bottles. All water used for cleaning and rinsing of plastic ware and mixing of reagents was first passed

through a Milli-Q^{TM} Water System at 18 μohms ("Q water"). Nitric acid used in water analyses was either distilled using a sub-boiling quartz still ("ultra-pure") or was Baker Ultrex^{TM} grade.

Nalgene$^®$ plastic ware was used for collection and storage of water samples was soaked in concentrated Baker$^®$ hydrochloric acid (HCl) for 24 hours, rinsed 3 times with Q water then filled with 1% ultra-pure nitric acid (HNO$_3$) solution and allowed to stand for a minimum of 5 days. These containers were then rinsed 3 more times with Q water and then filled with Q water. Such long term exposure to cleaning acids may not be needed if the temperature of acid solution is increased to ~ 60°C (Boyle and Heusted, 1983). The Q-water filled containers were placed in plastic bags and the bags sealed. During the cleaning procedure the sample containers were handled by individuals wearing clean vinyl or polythylene gloves. This was also done to minimize contamination. All cleaning was conducted in a hood. The bagged containers were stored in plastic garbage bags in a clean storage area within the laboratory until ready for use. The Q-water was decanted from the containers immediately before the containers were used for sample preparation or storage.

The teflon bailer and filtering apparatus were cleaned in concentrated nitric acid. Between uses, the filter on systems were rinsed in diluted (~ 10%) nitric acid and then rinsed copiously with Q water.

Sample Collection

Groundwater samples were collected from previously drilled wells and piezometers using a teflon bailer. This device was purchased commercially from the Cole-Palmer Instrument Co. The bailer has a 7/8" O.D. and is 3' long. Samples were immediately transferred from the bailer to a precleaned sample container. The samples were rapidly transported to our field laboratory (an open-sided garage lent to us by the Cheetham Salt Works) on the western-central shore of Lake Tyrrell. The samples were placed inside a N$_2$-filled glove bag and filtered. After filtration and while still in the glove bag, sub-

samples were divided into various aliquots using micropipettes.

The N$_2$ filled glove bags were utilized for two important reasons. Because hoods were not available to us at our field laboratory, the glove bags were used to minimize airborne contamination during the filtration step. In addition, many of the groundwater samples encountered in this study were suboxic to anoxic with extremely high Fe^{2+} concentrations. The filtrations were conducted under the inert N$_2$ atmosphere in the glove bag to minimize any oxidation artifacts (Loder et al., 1978; Lyons et al, 1979). The oxidation of Fe^{2+} is extremely rapid under atmospheric conditions so that if accurate dissolved Fe data are to be obtained from reducing waters this precaution must be taken. In addition, due to the fact that FeOOH is utilized analytically for quantitative removal or scavenging of dissolved trace metals from water samples, if care is not taken to prevent Fe$^2 \rightarrow$Fe^{3+}OOH, the possibility exists for the loss of other trace metals from solution.

Teflon filtering units (Cole-Palmer Instrument Co.) were utilized to filter the groundwater samples. Water was decanted into the units from the collection bottle while in the N$_2$ filled glove bag. Nuclepore^{TM} membrane filters were used with the teflon filtering units. The filters had previously been soaked in ~ 1% v/v ultra pure nitric acid solution to minimize metal loss and/or contamination (Truitt and Weber, 1979). Sample containers filled with Q water had previously been placed in the glove bag. When the sample had been filtered, the Q water was decanted from these precleaned Nalene^{TM} bottles and the subsamples micropipetted into them. The samples to be utilized for Fe$_T$, Mn, Pb, Cu and analysis were then acidified to ~ 1% v/v with ultra pure nitric acid. The acidification step was undertaken to minimize metal adsorption onto container walls (Subramanium et al., 1978). The acid cleaning of containers is needed to remove surface contamination but it can "activate" adsorption sites on the containers so that metal can easily adsorb (Batley and Gardner, 1977). The addition of strong acid maximizes the H$^+$ concentration in solution, displacing any metal adsorbed onto the

container. Finally, the sample vessels containing the acidified samples were placed into plastic bags and stored in a cool, dark and clean place until they could be shipped back to the University of New Hampshire via air freight. The bagged samples were placed into large plastic garbage bags and finally into ply-board foot lockers for shipment.

Sample Storage

When the samples arrived at UNH they were removed from their bags and placed in a Class 100 laminar flow clean bench until analyzed. The clean bench minimized any airborne particle contamination coming into contact with the sample containers. The samples were only handled by individuals wearing either vinyl or polyethylene gloves. In all cases, samples were never placed in contact with the following materials: rubber, tygon tubing, paper tissues, and metal and gloves containing talcum powder. These are all known potential contaminants. Although the laminar flow clean bench minimizes aerosol contamination (extremely important for Pb), contamination from other items or sources must be evaluated. For example, many plastic products like pipette tips can contain Zn or Cd. Therefore, pipette tips should either be cleaned or at least evaluated as a potential source of contamination prior to use.

Sample Analyses

Water samples were analyzed for Cu, Pb and Zn by flameless atomic absorption spectrophotometry (FAAS) using a Perkin-Elmer model 2280 Atomic Absorption Spectrophotometer equipped with an HGA 400 graphite furnace, AS-40 auto-sampler and deuterium background corrector.

In order to analyze these metals accurately and precisely, it was necessary to remove them from the hypersaline sample matrix (Weisel et al., 1984). Cu, Pb and Zn were coprecipitated with ferric hydroxide after the method of Weisel et al. (1984), as modified for hypersaline samples by Welch et al. (in review). A detailed explanation of our technique is not warranted here for it will appear elsewhere. Standard additions were

also conducted on a number of samples in order to check the method. Kling et al. (in review) have also used this technique for Al, Mn and Ni analysis. Five ml of sample were combined with 20 ml of 1% ultra-pure HNO_3 and 100 μl of 1M Alfa Products[®] iron (III) nitrate. The pH was adjusted to 7.5-8.0 using 30% Ultrex[®] ammonium hydroxide (NH_4OH), causing precipitation of the metals with ferric hydroxide (FeOOH). This precipitate was collected on a 47 μm Nuclepore[®] filter using a precleaned Millipore[®] filtration apparatus, then redissolved in 5 ml of 10% ultrapure HNO_3 and kept for analysis. The filters were cleaned by first soaking them for 2 days in 5% ultra-pure HNO_3, then rinsing them 6 times. They were finally stored in Q water until needed. The filtration apparatus was rinsed in 10% Baker[®] HNO_3 and rinsed 3 times with Q water between uses. Samples were diluted into the linear range of the standard curves using 1% ultra-pure HNO_3.

The dilutions differed for each element: 10:1 for Pb and Cu and 25-100:1 for Zn. All Al, Pb and Zn standards used were made from 1000 μg/kg VWR[®] standard solutions. All other standards were made from 1000 μg/kg Alfa Products[®] standard solutions. Ni standards were prepared in 10% ultra-pure HNO_3 to facilitate atomization in the furnace. All other standards were made in 1% ultra-pure HNO_3. The FAAS parameters utilized for all these metals are shown in Table 1. Recovery experiments run by Welch et al. (in review) indicate average recoveries of 89%, 89%, 79% and 119% for Cu, Pb, Zn and Mn, respectively, in concentrations between 0.5 and 3.0 M NaCl. Weisel et al. (1984) indicate recovery efficiencies of 85% for Al in seawater of pH 7.5 and 100% recovery of Pb in seawater of pH 6.0 We conducted no recovery experiments for Ni. Detection limits of this technique are 0.5, 1.0, <0.2μgL^{-1} for Pb, Cu and Zn respectively. Small volume samples were utilized due to the fact that the low pH of RGW suggested that dissolved metal concentrations could be high. This was indeed the case. The technique outlined here could easily be utilized for large volume samples and with smaller dilution volumes in order to measure lower concentrations of trace metals in groundwater. For example, Weisel et al. (1984) utilized 250 ml seawater

samples, redissolved the FeOOH precipitate with 2 ml of nitric acid and then analyzed these without dilution.

Fe_T and Fe^{2+} were determined in the field using the ferrozine-colorimetric technique (Murray and Gill, 1978). Mn was determined via FAAS after a 10:1 dilution with Q-water. The analytical variation of a number of Lake Tyrrell samples is shown in Table 2.

Due to the low volatility of Ni, sensitivity for this metal was low. In addition, the graphite tubes quickly became contaminated with Ni and had to be replaced after every 20-25 samples and standards. Al also showed a tendency to absorb into the graphite tubes, causing an increase in blank concentrations over time. Tubes were replaced after analysis of 50-60 samples and standards. An additional problem was encountered with Zn. It was determined that when samples were precipitated onto year-old filters they became contaminated with Zn with blanks as large as 0.2 μM. The source of contamination was determined by testing of the filter storage (dilute acid) as well as the reagents.

If samples are stored in clean containers, acidified and placed in a "clean environment," contamination should be minimal. Boyle and Huested (1983) have shown that strict clean room techniques are not needed to make ultra trace Pb measurements in natural waters. However, the use of Class 100 laminar flow clean benches is now thought to be imperative in maintaining sample integrity during sample manipulation. Our samples were stored in the clean bench while being analyzed. After analysis they were again bagged and placed in a cool, dark and clean location.

Blank Determinations

Blank determinations are the most important measurements to be made. While we were in the field collecting water samples an aliquot of Q water was filtered and processed as a sample once a day. This aliquot was approximately the same size as the sample. This was done on four days. The results are shown in Table 3. Our Pb blanks were all below the detection limit of

our analytical technique while the Cu and Zn blanks were measurable. The low Pb blanks indicate that there was little to no aerosol contamination of our samples. Small volume samples inherently have the most potential for contamination (Brewer et al., 1974; Brewers et al., 1976; Patterson and Settle, 1976). Because of the high concentrations of NaCl in these waters of the Lake Tyrrell system, some preconcentration step was needed to remove the trace metals from the sample matrix, yet due to the high trace metal concentrations in the waters only small sample sizes could be utilized for analysis. These, in turn, had to be diluted (see above discussion). Therefore our Cu and Zn blanks were high probably due to the small volume of the sample as well as to the increased sample manipulation needed to remain in the linear working range of the instrument. This contention is supported by the fact that, in general, reagent blanks yielded Pb, Cu and Zn values below the detection limit of the method. Because of these issues, we feel that these blanks (Table 3) should be considered maxima. (For example, we have previously reported much lower procedural blanks for Cu from our laboratory, Lyons et al., 1980). There are no systematic trends in these blanks as the highest Cu blank is from the last day while the highest Zn blank is the first day. The two highest Cu blanks, however, are associated with the two highest Zn blanks. It is not uncommon to experience relatively high Zn blanks. Numerous investigators have documented the difficulty in minimizing Zn in their blanks (Struempler, 1973; Sturgeon et al., 1980; Rasmussen, 1981; Paulson, 1986). The blank values were subtracted from our samples in order to obtain the final Pb, Cu and Zn concentrations (Table 4). We feel that any trace metal data should be accompanied with a detailed discussion of how blanks were determined as well as what they are.

RESULTS

As noted by Macumber (1983), and outlined above, the water from the Lake Tyrrell system can be divided into three main regions: the acidic regional groundwaters (RGW), the reflux brine (RB) and the neutral Wahpool-Timboram (NWT) brine. The RGW

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have very low pH's (2.9-3.9). The variation of Fe, Mn, Pb, Cu and Zn concentrations of these waters help to further divide the RGW into a northern and a southern group (Fig. 1) and (Table 4). The northern group has slightly higher Pb, Cu, Zn and Mn concentrations. A high percentage of the dissolved Fe_T in the RGW is Fe^{3+} (Lyons et al., in review). The differences between the northern and southern RGW trace metal concentrations indicate subtle differences in aquifer composition, heretofore unidentified. The Parilla Sand does contain numerous heavy mineral bands (Macumber, 1983). The variation in this component of the aquifer probably has important effects on the trace metal concentrations of the RGW.

The RB can either be anoxic with extremely high dissolved Fe_T and very low Pb, Cu and Zn concentrations or be oxic with low Fe_T and higher Pb, Cu and Zn values. The NWT waters have the highest pH's of the system and have relatively low Fe_T, Mn, Cu, Pb and Zn concentrations (Table 4).

The oxidic RGW from the Tyrrell system have higher concentrations of Cu, Pb and Zn than unpolluted groundwater (e.g. Jickells et al., 1986; Jacobs et al., 1988). This is due to their extremely high Cl-content and low pH. Chloride forms strong complexes with most trace metals and high H+ concentrations increase the solubility of metals. Taylor et al. (1984) have found groundwaters with a higher pH and Lower Cl-concentration within a few 100 km of the Lake Tyrrell region also with much lower metal concentrations($Cu \approx 1 \mu gL^{-1}$; $Pb \approx 7 \mu gL^{-1}$; $Zn \approx 60 \mu gL^{-1}$).

The three water types are related in that RGW has evolved into RB and NWT water by either discharging onto the lake floor where it is further evaporated and mixed with surface lake water and "refluxed" back into the lake sediments or, in the case of NWT, by "refluxing" through the Lake Timboram-Wahpool system. In places along the lakes' edges the RGW overlies the RGW. The RGW discharges onto the lake surface on the W and SW portions of the lake while NWT discharges along the E side of the lake. Macumber (1983) has shown that the ground-

water brines in the Tyrrell Basin have accumulated within the last 32,000 years. Although they have differing Cl-concentrations, these three brines are similar in major element composition and have, in general, evolved as a chemical continuum (Long et al., in review). Our data show, however, that as these waters have evolved and their Cl-content increased by evapoconcentration, their trace metal geochemistries have changed. The major factors in the changing concentration of trace metal in the Tyrrell system are apparently pH and Eh. It is obvious that the low pH waters can carry high concentrations of Pb, Cu and Zn and also high Fe^{3+}. The reducing waters of the reflux brines have lost much of their Pb, Cu and Zn probably due to sulfide mineral precipitation within the aquifer and Fe^{3+} is converted to Fe^{2+}. The more oxidizing reflux brines have higher Pb, Cu and Zn concentrations due to the lack of removal via metal-sulfide formations.

CONCLUSIONS

In order to obtain trace metal data that is of top quality great care must be taken during sample container preparation as well as sample collection, storage and analysis. Procedural and reagent blanks should be determined and presented before the data from monitoring programs can be adequately evaluated. Knowledge of potential contamination problems should be understood before any samples are collected. The need of clean sample containers, sampling apparatus, water acid and storage space is essential for meaningful data collection. In this paper we have presented a detailed description of how we have approached these problems utilizing a study of Fe, Mn, Pb, Cu and Zn in groundwaters from the Lake Tyrrell region, Victoria, Australia. The study has documented subtle changes in the trace metal content of the regional groundwater in the region that is undoubtedly due to inhomogeneities in the aquifer material. In addition, the three major groundwater types in the area which had previously been differentiated by their pH and TDS also have different mean trace metal concentrations.

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CONFIDENCE INTERVALS FOR THE MEAN USING TRACE LEVEL WATER QUALITY DATA

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ABSTRACT

As efforts are made to improve the information obtained from water quality monitoring systems, the use of statistics is finding wider application in the analysis of water quality data.   Water quality data records that contain "not detected" (ND) or "less than" (LT) are a mixture of numerical and non numerical sampling results and are difficult to analyze using standard statistical methods. In recent years there have been a number of procedures suggested to statistically analyze data records with NDs and LTs. Each of these attempts to overcome the loss of information that accompanies the ND or LT. This paper suggests that the actual reading from the laboratory be placed in the data record along with a statement of uncertainty. This modifies the ND and LT concept and, it is suggested, opens the way for more meaningful statistical analysis of water quality data. Three such data analysis methods are presented and compared with a current method which incorporates the ND and LT concepts. While these methods improve the statistical analysis of trace level data, they may yield negative variance estimates. Further work is needed to define the use of such water quality information within water quality management decision making.

I. Introduction

Trace level water quality measurements are often reported "not detected" (ND) or "less than" (LT). Not detected and LT are impor-tant concepts when individual measurements are interpreted, but are less informative than a numerical result and statement of uncertainty (Gilliom et al. 1984; Gilbert and Kinnison, 1981; Porter et al. 1988). In addition, methods for overcoming the ND and LT limitations often make assumptions about how the unknown numerical results below the ND and LT behave. Such assumptions are unnecessary when the numerical result provides the exact behavior. Moreover, methods for analyzing numerical results are simple and familiar in comparison to methods for analyzing censored data.

Statistical properties of measurements differ from those of the (unobservable) true process in ways which affect the selection and outcome of statistical methods. Variability caused by measurement reduces the ability to detect changes in a process and obscures correlation and seasonal patterns. In addition, when observation error is normally distributed, measurements are more symmetric than the underlying process (Porter and Ward, 1989).   Statistical methods for normally distributed data may be applicable to measurements when they would not be appropriate for the process observed without error.

Trace level measurements are inherently imprecise. Analysts censor data to protect the integrity of numerical results.   Criteria based on measurement precision form the basis of reporting conventions for trace level measurements. For example, the American Chemical Society (ACS, 1983) recommends the following:

"not detected" - the analytical response is less than the limit of detection (LOD),

"detected" - the analytical response is between the LOD and the limit of quantification (LOQ - the "region of less-certain quantitation"),

numerical result - the analytical response is greater than the LOQ.

However, trace level measurements contain information even if they are very imprecise. When data have many imprecise results, the accumulation of information can be important (Porter et.al, 1988; Currie, 1988). Therefore, improvement in data analysis results when data are not censored.

Statistical methods useful for interpreting trace level measurements will generally be simple relative to those for censored data, but two problems need to be addressed. Measurements below the LOQ are imprecise and do not faithfully reproduce the statistical characteristics of the underlying process. (This is a greater problem for censored than for uncensored data). It is important to realize that statistical methods lead to inferences about measurements which may not hold true for the process being monitored. The same analysis applied to observations made without error may yield different conclusions.

A second problem is that of negative results, which may occur when signal errors are normally distributed. The ASTM (1983) points out that ". . . if the constituent of interest is not present, one would expect negative results to occur as often as positive." They suggest that "in order that valid inferences may be made from data sets, it is important that negative results be reported as such." Negative results may lead to confidence intervals which overlap zero. Obviously, true concentrations cannot be less than zero, but negative results lead to difficult problems of interpretation. For example, a confidence interval which overlaps zero isn't correct, but it's true size and location are not known. (The problem is

worse for confidence intervals produced by censored data).

The problem of negative results can be addressed through examination of the probability space of measurements and conditioning the outcome of statistical tests on the basis of what is possible. For example, the knowledge that the true mean of a process must be positive can restrict values of Student's t statistic.

Further improvement in water quality data analysis is possible when variability caused by measurement is separated from process variability. Variance correction techniques subtract components of variance due to measurement from the sample variance.

In this paper, construction of a confidence interval for the mean of a lognormal distribution is examined using three different approaches. A method for censored data is described briefly and, since such methods are in common use today, held in comparison to three more informative methods: (1) a confidence interval based on Student's t statistic and formed with numerical results, (2) a Bayesian correction to Student's t statistic, and (3) a variance correction method. Each method is described, a worked example is provided, and some properties of each method are given.

II. Statistical Properties of Measurements

Consideration of the effect of measurement on data can lead to better selection of statistical methods. For this discussion, the water quality "process" will be, simply, a lognormally distributed constituent of water (X_p), and concentration estimates will be based on measurements of samples and standards.

Measurement is the conversion of chemical information to a signal (say a digital voltage readout). Calibration is the transformation of analytical signals into estimates of concentration. When the relationship between chemical concentration (X) and analytical signal (S) is linear, the calibration function is given by:

$$S = B_o + B_1 X + e_s \tag{1}$$

$$e_s \approx N(0, k_o + k_1 X)$$

where B_o and B_1 are the true intercept and slope, respectively, of the signal-concentration relationship, X is true sample concentration, and e_s is random signal error. Near the limit of detection, the variance of e_s is linearly related to concentration, with k_o and k_1 the intercept and slope, respectively, of this relationship (Prudnikov, 1981; Prudnikov and Shapkina, 1984).

The slope and intercept (B_o and B_1) are estimated from a calibration experiment which is the measurement of samples with known concentration. Calibration design is the choice of the number and spacing of standard samples used to estimate B_o and B_1. A two point end point design has minimum variance but cannot detect non-linear calibration functions; therefore, equally spaced, equally weighted calibration designs are often used in practice (Fig. 1).

Estimates (X_m) of true process concentrations (X_p) are given by:

$$X_m = (S - b_o)/b_1 \tag{2}$$

Where b_o and b_1 are estimates of B_o and B_1, respectively, derived from the calibration experiment. When signal variance is related to concentration, weighted least squares should be used to estimate B_o and B_1.

When signal error (e_s) is normally distributed, X_m is a ratio of two correlated, normally distributed quantities. The mean and variance do not exist for ratios of normal quantities, but a 1st order Taylor series expansion of X_m (or propagation of errors, POE) has many of its characteristics (Porter and Ward, 1989). The resulting probability density function (PDF), denoted $f(POE/p)$, has a mean and variance. If signal error (e_s) is normally distributed, then X_m, given the true value (X_p) can be assumed to be normally distributed with mean and variance, is given by:

$$f(POE/p) \approx N\{X_p, \sigma^2(e_s)/(\kappa B_1^2) \tag{3}$$

$$+ [\sigma^2(b_o) + 2\sigma^2(b_o b_1)X_p + \sigma^2(b_1)X_p^2]/B_1^2\}$$

The term $f(POE/p)$ refers to the PDF of a measurement given a sample from a process. The term POE refers to the approximation of X_m by a Taylor series; $\sigma^2(e_s)$ is the variance of random signal error; and the $\sigma^2(\cdot)$ terms are the variances of the parameter estimates (variances of b_o, b_1 and the covariance of b_o and b_1). The variance of $f(POE/p)$ can be written in terms of X_p:

$$Var(POE/p) = r + sX_p + tX_p^2 \tag{4}$$

where r, s, and t are constants given by:

$$r = (k_o/\kappa + \sigma^2(b_o))/B_1^2 \tag{5}$$

$$s = (k_1/\kappa + \sigma^2(b_1,b_o))/B_1^2$$

$$t = \sigma^2(b_1)/B_1^2$$

The message of this development is that the variance of measurements is influenced by calibration design (Fig. 2).

A limit of detection defined by ACS (1983) is three times the standard deviation of the analytical signal of a blank measurement. The standard deviation is considered known when many (say 30) measurements are used in its determination.

$$LOD = 3 \cdot \sigma(e_s) \text{ when } X_p = 0 \tag{6}$$

$$= 3 \cdot k_o^{1/2}$$

The LOQ is the minimum concentration which a reported numerical result ought to possess. The LOQ can be defined as the concentration corresponding to a signal which has a relative standard deviation (RSD) of 10%:

$$RSD = \sigma(e_s)/S \tag{7}$$

$$0.10 = (k_o + k_1 \cdot LOQ)^{1/2}/S_{LOQ}$$

190
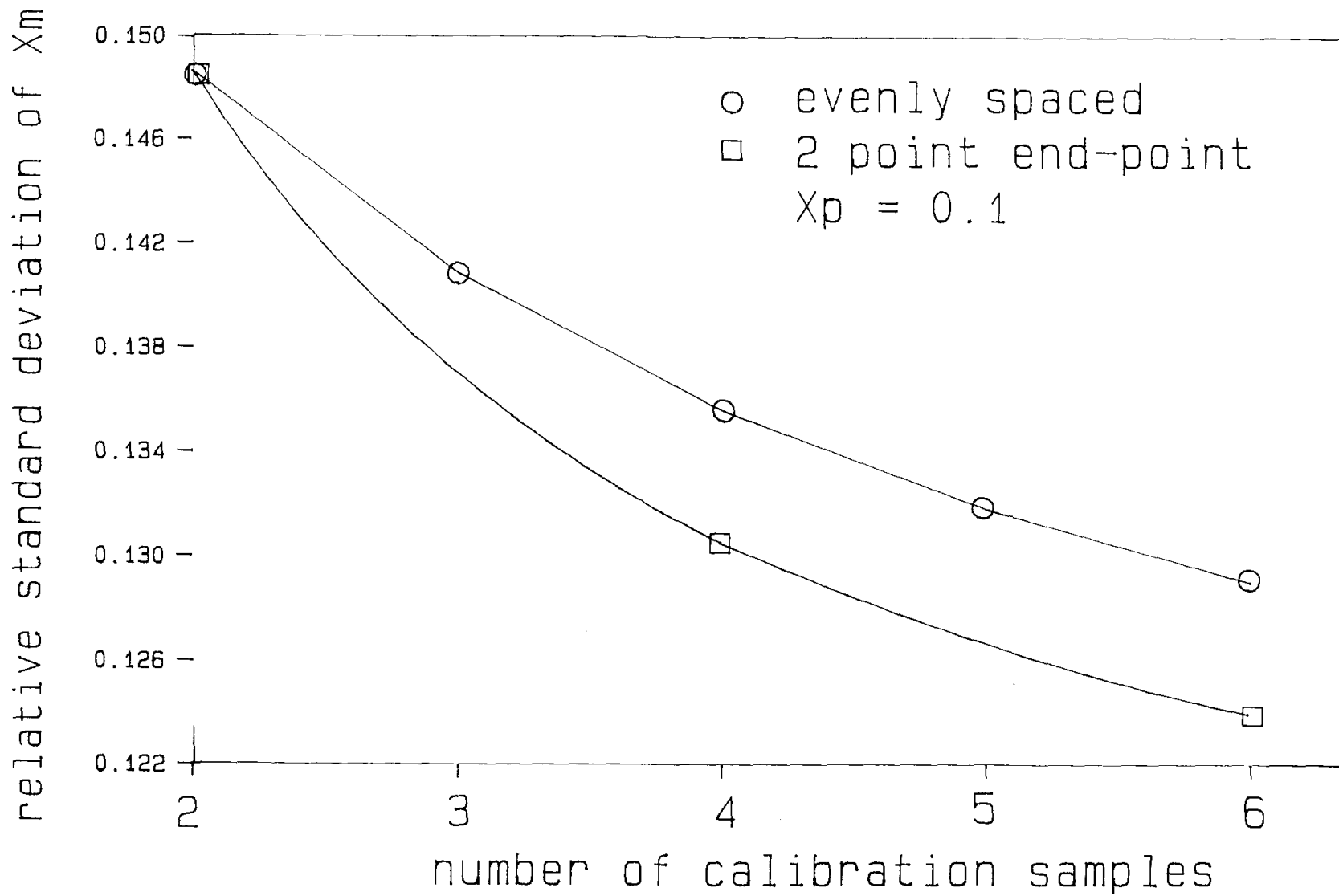
Figure 1.   Effect of calibration design on measurement precision

Population CV = 0.2, LOD/LOQ = 0.3

○   Cal.Des. = [1 @ 0, 1 @ 1]; fc = 0.1

●   [1 @ 0, 1 @ 1]; fc = 0.9

□   [12 @ 0, 12 @ 1]; fc = 0.1

△   [12 @ 0, 12 @ 1]; fc = 0.9

---- LOD

analyte concentration
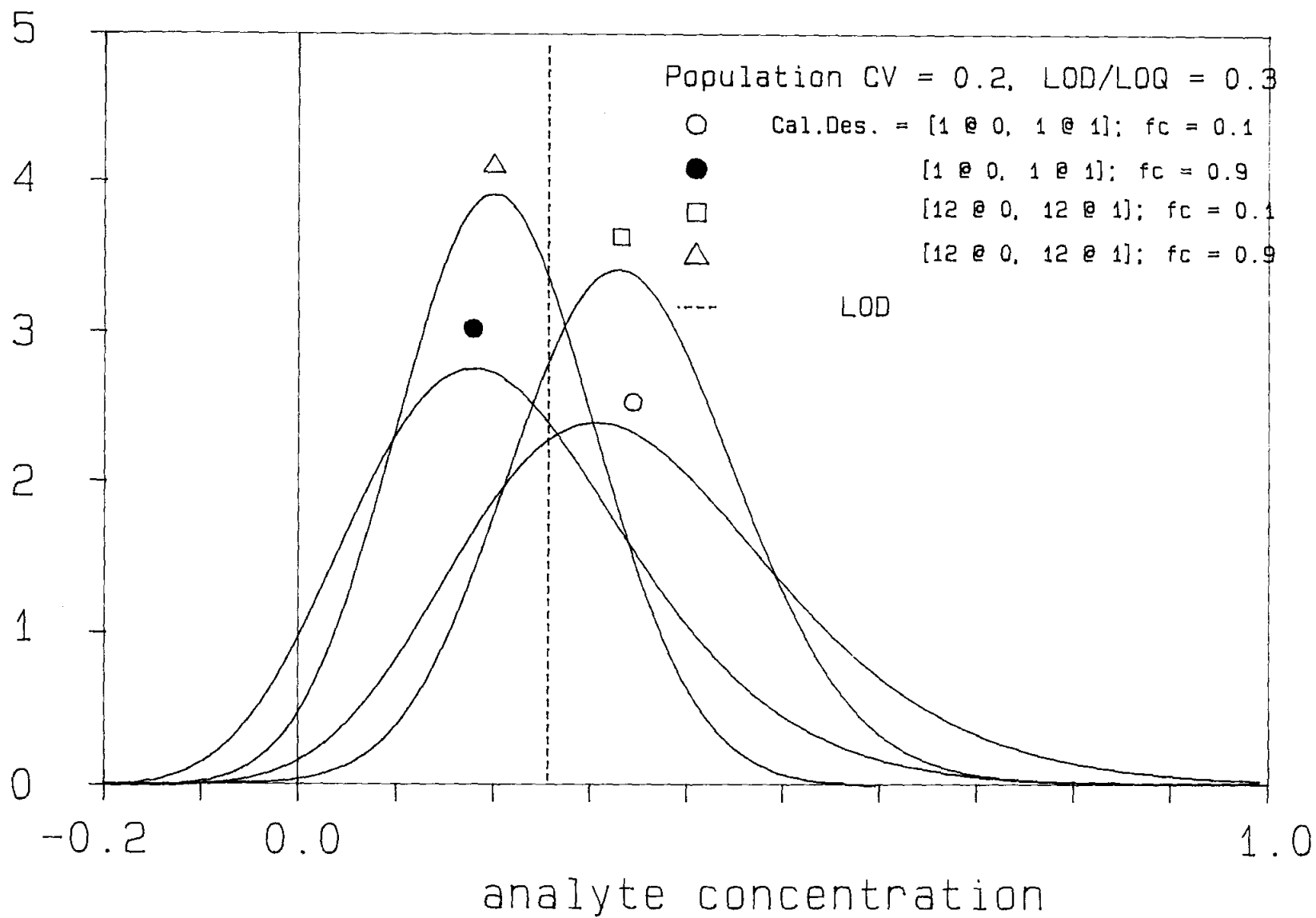
Calibration and Measurement *PDF*'s

Figure 2.   Effect of calibration design on measurement PDF's

where S_{LOQ} is the signal produced by a sample with concentration LOQ. The concepts of LOD and LOQ as they relate to the RSD are illustrated by Fig. 3.

The ratio of concentrations corresponding to LOD/LOQ summarizes a great deal of information about a measurement process. In terms of other measurement parameters,

$$X_{LOD}/X_{LOQ}=0.06 \cdot [R^{1/2}+(R + 0.04)^{1/2}]^{-1} \quad (8)$$

where $R = k_I^2/(k_o B_I^2)$.

The PDF of measurements, a convolution of the underlying process and observation error, is given by:

$$f(POE) = \int_o^\infty f (POE/p) \cdot f_p dX_p \quad (9)$$

where f_p = process PDF

$$= (2 \cdot \pi)^{-1/2}(\sigma_p X_p)^{-1} \exp\{-0.5$$

$$[\ln X_p - \mu_p)/(\sigma_p)]^2\}$$

X_p = water quality random variable

α_p = process mean

$$= \exp(\mu_p + \sigma_p^2/2)$$

β_p^2 = process variance

$$= \exp(2 \cdot \mu_p + \sigma_p^2) \cdot [\exp(\sigma_p^2)-1]$$

$$Var[f(POE)] = \sigma_m^2 \quad (10)$$

$$= r+s\alpha_p+(t+1)\beta_p^2+t \cdot \alpha_p^2$$

III. **Uncensored estimates of the mean**

The asymptotic relative efficiency (ARE) is the ratio of the variances of two estimators whenthe sample size approaches infinity. The relative size of two two confidence intervals derived from these estimators is proportional to the ARE. The ARE of the sample mean from a lognormal distribution relative to the

sample mean of measurements from that distribution is approximated by:

$$ARE = [\alpha_p(\sigma_p^2+\sigma_p^4/2)]/[\alpha_m(\sigma_m^2+\sigma_m^4/2)] \quad (11)$$

(based on the maximum likelihood estimation (MLE) of Finney (1941) described in Aitchison and Brown, 1957).

The ARE was used to compare a method for censored data and the sample mean available when all numerical results are reported. The ARE for both relative to error free observations were computed.

As the number of calibration samples approaches infinity the POE approximation becomes:

$$\alpha_p = \alpha_m \text{ and} \quad (12)$$

$$\beta_m^2 = k_o + k_1\alpha_p + \beta_p^2.$$

The ARE for censored data is obtained by estimating the location and scale parameters of a lognormal distribution (μ and σ) using MLE and converting to an estimate of the mean and variance using the expression $\hat{\alpha}$ = $\exp(\hat{\mu} + \hat{\sigma}^2/2)$ and $\hat{\beta}^2=\exp(2 \cdot \hat{\mu} + \hat{\sigma}_p^2) \cdot [\exp(\hat{\sigma}_p^2)-1]$ (Aitchison and Brown, 1957). The variances of $\hat{\mu}$ and $\hat{\sigma}$ are given by (Cohen, 1961).

$$\text{Variance of } \hat{\mu}_m = K(\mu_m) \cdot /n \quad (13)$$

$$\text{Variance of } \hat{\sigma}_m = K(\sigma_m) \cdot \sigma_m^2/n$$

$$\text{Covariance of } (\hat{\sigma}_m, \hat{\mu}_m) = K(\mu_m \cdot \sigma_m) \cdot \sigma_m^2/n$$

The values of the K(·) (found in Cohen, 1961) depend on the degree of censoring. The variance of $\hat{\alpha}_p$ can be approximated by a propagation of errors argument based on the expression for $\hat{\alpha}$ given by (14):

$$\text{Variance of } \hat{\alpha}_p \approx \alpha_p^2 \cdot \sigma_m^2[K(\mu_m)+\sigma_m^2 K(\sigma_m)$$

$$+ 2\sigma_m K(\mu_m \cdot \sigma_m)]/n \quad (14)$$

The censored data method is always less efficient than estimates using uncensored data (Fig. 4). For small samples, the differences would be greater.
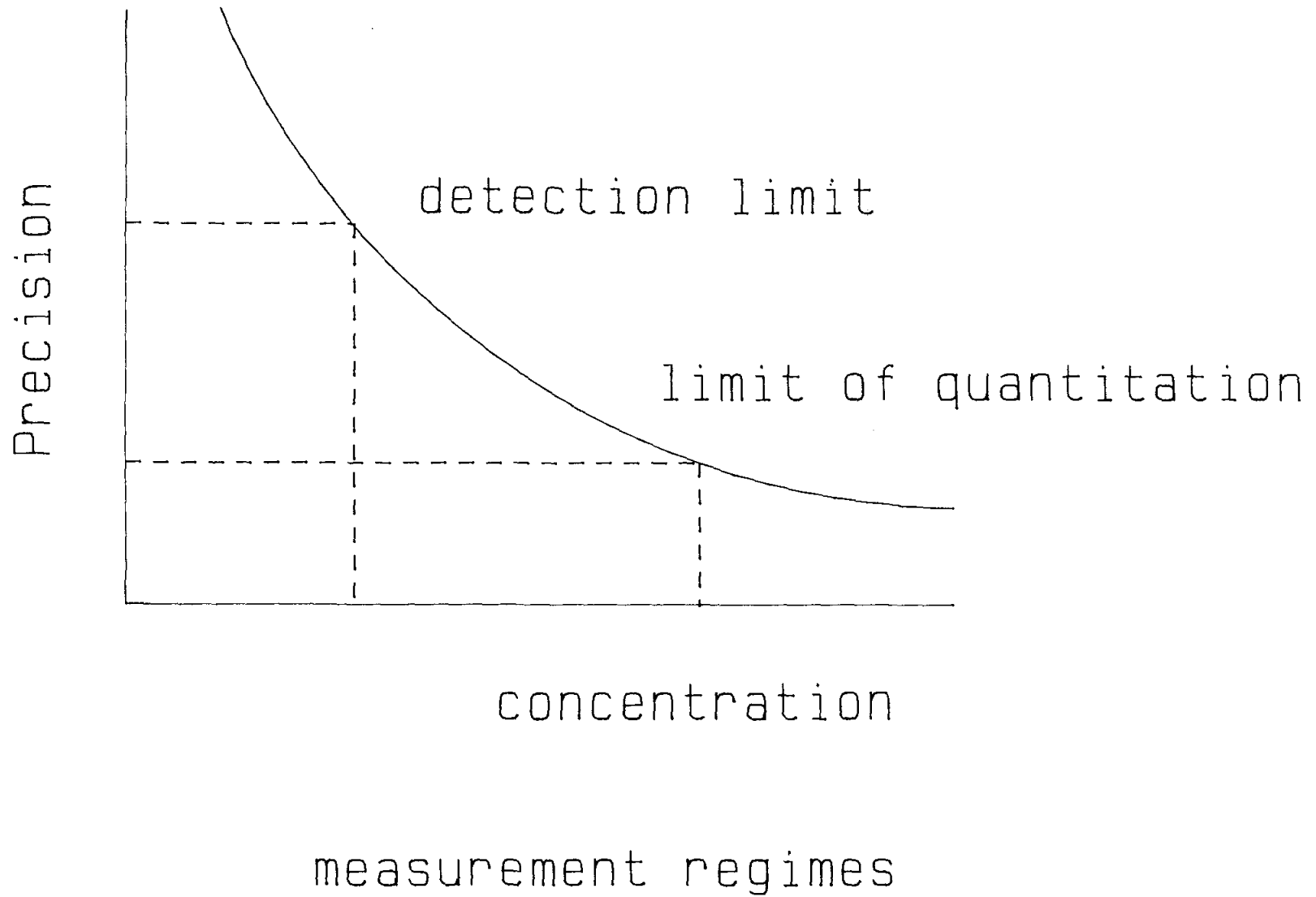
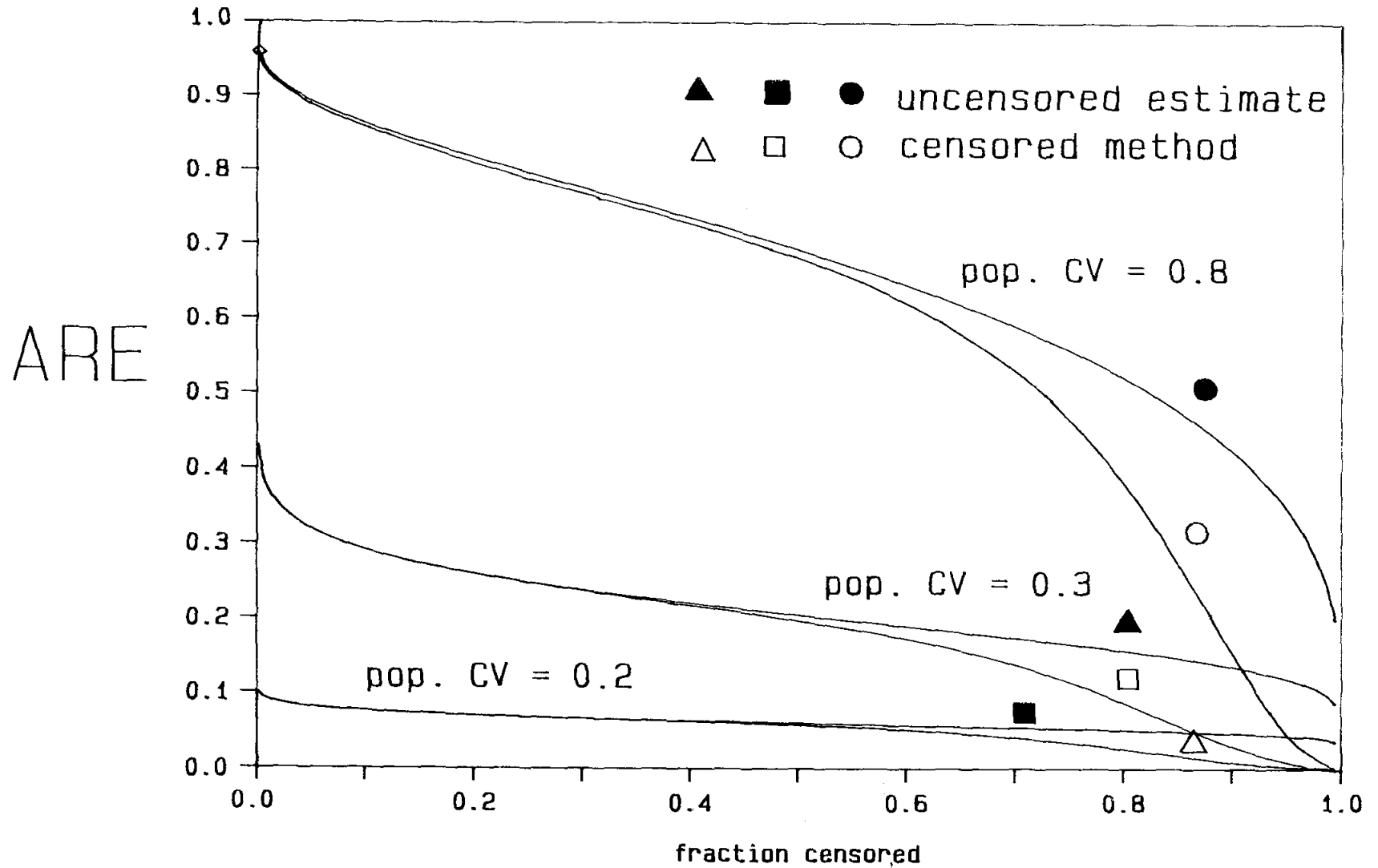Figure 3.   Precision criteria for censoring

Figure 4. *Efficiency of the MLE estimate of the mean for a
lognormal distribution relative to error-free
observations; censored vs. uncensored data*

Computation of a confidence interval for censored data is described by Schmee et.al (1985) and an example of its use can be found in Table 1.

IV. Bayesian Confidence Intervals

Confidence intervals based on uncensored measurements may overlap zero. However, a Bayesian estimate of a confidence interval for the mean makes use of prior information about the true mean. For example, consider a confidence interval based on Student's T statistic given by:

$$t = (\bar{X}-\mu)/(S/\sqrt{n}) \tag{15}$$

When the true mean (m) is greater than 0, t cannot exceed $\bar{X}/(S/\sqrt{n})$. A confidence interval, given this restricted range of t, is found by solving:

$$1 - \alpha = \int_{TL}^{TU} f(t,n\text{-}1)dt \Big/ \int_{-\infty}^{TM} f(t,n\text{-}1)dt \tag{16}$$

for TL and TU, where (TL, TU) are lower and upper bounds on Student's t which will result in 1-α coverage for the restricted t distribution, TM is the maximum allowable t statistic $[\bar{X}/(S/\sqrt{n})]$, and $f(t,n\text{-}1)$ is the PDF of Students t for n-1 degrees of freedom. It is simplest to choose TL and TU which provide equal weight to the tails.

The Bayesian confidence interval is always smaller than a confidence interval based on an unrestricted t statistic and will never overlap 0 (Fig. 5). When the sample standard error is much larger than 0, both confidence intervals are nearly the same size. Tables based on equation (16) are easily constructed using tables or software which provide tail areas for Student's t distribution. Solubility considerations, which place an upper limit on concentration, may also be incorporated into this approach. A numerical example can be found in Table 2.

V. Variance Correction Methods

A. Improved degrees of freedom

Random measurement error may be estimated and removed from the total variance of measurements. To illustrate, consider a true population variance based on the POE estimate (equation 10):

$$\hat{\beta}_p^2 = [\hat{\sigma}_m^2 - (r + s\cdot\bar{X}_m + t\cdot\bar{X}_m^2)]/(t + 1) \tag{17}$$

Satterthwaite (1946) and Gaylor and Hopper (1969) address a problem similar to that suggested by equation (17), the distribution of linear combinations of variance estimates (sums of squares). A linear combination of variance estimates can be approximated as chi-squared (χ^2) with "improved" degrees of freedom (Satterthwaite, 1946); e.g.,

$$\hat{\sigma}^2 = a_1\hat{\sigma}_1^2 + a_2\hat{\sigma}_2^2 \approx \sigma^2\chi_f^2/f \tag{18}$$

where $f = (a_1\hat{\sigma}_1^2 + a_2\hat{\sigma}_2^2)^2/[(a_1\hat{\sigma}_1^2)^2/f_1$

$$+ (a_2\hat{\sigma}_2^2)^2/f_2]$$

and f_1 and f_2 are the degrees of freedom of the estimates $\hat{\sigma}_1^2$ and $\hat{\sigma}_2^2$, respectively. This estimate is valid for positive a_i (also see Satterthwaite, 1946; Mulrow et. al, 1988; and Welch, 1947).

Satterthwaite (1946) cautions against using equation (18) when some of the a_i are negative; therefore, Gaylor and Hopper (1969) examined negative a_i. Consider:

$$\hat{\sigma}^2 = \hat{\sigma}_1^2 - \hat{\sigma}_2^2 \tag{19}$$

The objective is to approximate ∂^2 by:

$$\hat{\sigma}^2 \approx \sigma^2\chi_f^2/f \tag{20}$$

$$\approx \sigma_1^2\chi_{f_1}^2/f_1 - \sigma_2^2\chi_{f_2}^2/f_2$$

and to approximate f by:

$$f = (Q\text{-}1)^2/ (Q^2/f_1 + 1/f_2)$$

where $Q = \hat{\sigma}_1^2/\hat{\sigma}_2^2 \tag{21}$

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Table 1. Calculation of confidence intervals using censored
and uncensored data

Data Used for Examples: Monthly groundwater analyses
1,1,2,2-Tetrachloroethene (mg/L)
Detection limit = 1.0 mg/L

	Result	
	Numerical	Censored
1	0.24	ND
2	-0.84	ND
3	-0.72	ND
4	2.05	2.05
5	0.03	ND
6	1.78	1.78
7	1.44	1.44
8	1.50	1.50
9	2.01	2.01
10	1.00	1.00
11	0.76	ND
12	0.41	ND
13	1.49	1.49
14	2.13	2.13
15	1.08	1.08
16	0.02	ND
17	0.00	ND
18	0.45	ND
19	-0.69	ND
20	0.08	ND
21	0.49	ND
22	-0.76	ND
23	0.48	ND

sample mean   0.627   0.789[1]

sample variance   0.880   0.672[1]

t(22, 0.975)   2.074

$\hat{t}(0.025,23,9)$[2]   -1.22

$\hat{t}(0.975,23,9)$[2]   0.47

Confidence Intervals:

censored   = [0.789+(-1.22)·(0.820); 0.789+(0.47)·(0.820)]
            = [-0.21; 1.17]

uncensored = [0.627-(2.074)·(0.938)/$\sqrt{23}$; 0.627+(2.074)·(0.938)/$\sqrt{23}$]
            = [0.22; 1.03]

1 maximum likelihood for censored normal samples
2 from Schmee et.al, 1985

limits on true mean

sample mean

Bayesian interval
Student's t interval
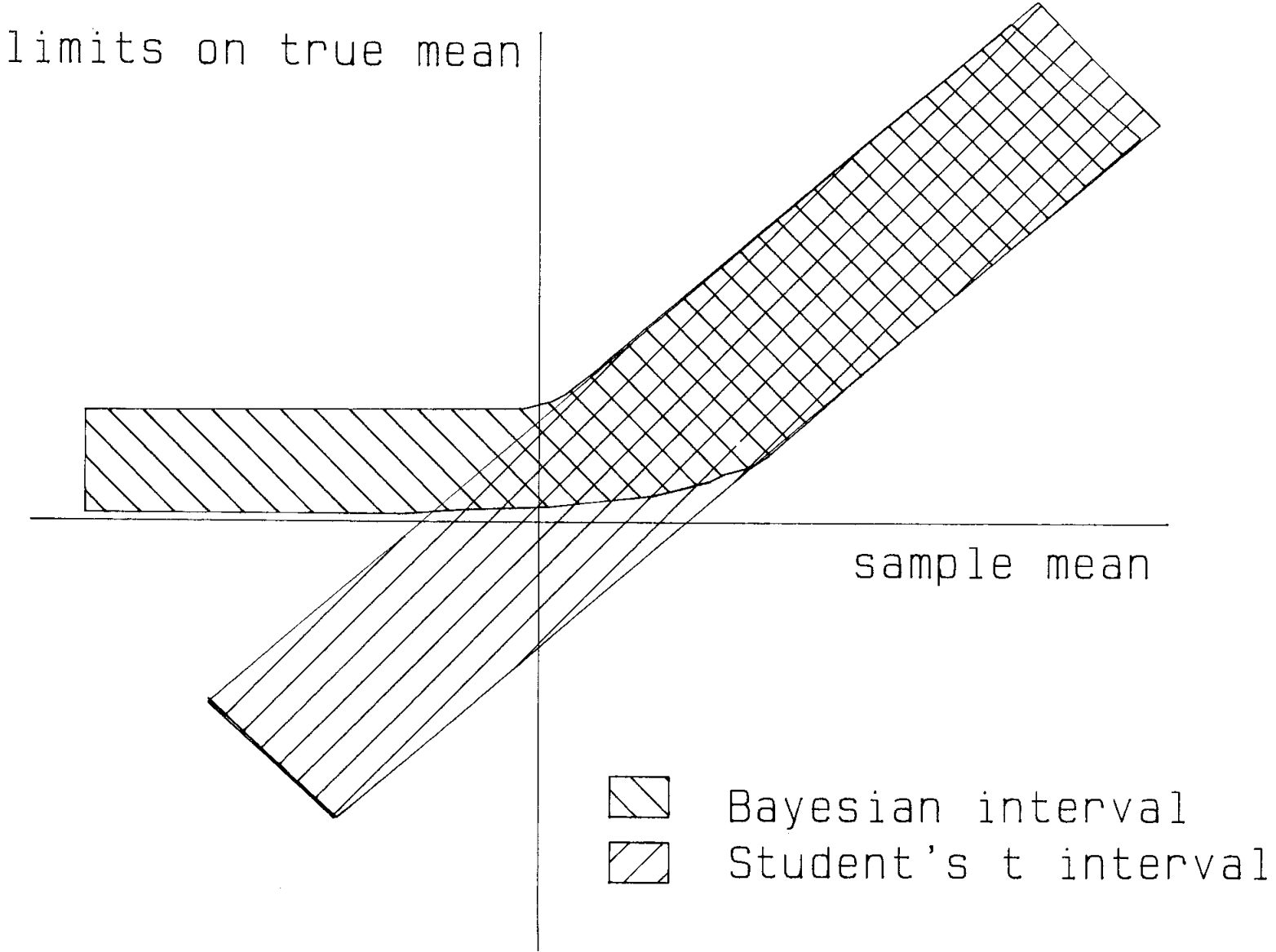
Figure 5.   Bayesian confidence interval

Table 2. Calculation of Bayesian confidence interval

$TM = \bar{X}/(S/\sqrt{n})$

$\quad = 0.627/(0.88/23)^{\frac{1}{2}}$

$\quad = 3.2055$

$CDF\ [t(22,0.99796)] = 3.2055$

$0.025 \cdot 0.99796 = 0.0.024949$

$0.975 \cdot 0.99796 = 0.0.973011$

$TL = CDF\ [t(22,0.024949)] = -2.07538$

$TU = CDF\ [t(22,0.973011)] = \quad 2.03639$

$CI = [\bar{X} - TU \cdot S/\sqrt{n},\ \bar{X} + TL \cdot S/\sqrt{n}]$

$\quad = [0.229\ ,\ 1.033]$

<u>In this case, not much difference from conventional Student's t</u>

Equations (20) and (21) are good approximations, with fewer than 2.5% negative $\hat{\sigma}^2$ results, if:

$$Q \geq F(f_2, f_1, 0.975) \cdot F(f_1, f_2, 0.50) \qquad (22)$$

for $f_1 \leq 100$ and $f_2 \geq f_1/2$, where F(a,b,p) is p^{th} percentile of the F distribution with a and b degrees of freedom. Note also that $0 \leq f \leq f_1$.

A new confidence interval for μ_p is given by:

$$CI = \hat{X} \pm t(1-\alpha, f) \cdot \hat{\sigma}_p/(n-1)^{1/2}, \qquad (23)$$

where $\hat{\sigma}_p^2 = \hat{\sigma}_m^2 - \hat{\sigma}^2(\epsilon)$

This confidence interval will usually be smaller than that given by the POE or Satterthwaite's improved degrees of freedom (SIDF) approach described by Mulrow et al.(1988). If data fail the criteria for negative results, it is suggested that f_1 and/or f_2 be increased by performing replicate analyses (Gaylor and Hopper, 1968).

The coefficient of variation of f is rather large. As f increases, the size of a confidence interval decreases, and $\hat{\sigma}_p^2$ will tend to increase. However, the confidence interval remains about the same size, given widely varying estimates of f (Gaylor and Hopper, 1968).

The approach of Gaylor and Hopper (1968) is valid when both variance estimates are distributed as chi-square (χ^2). (That is, X_p and ϵ are normally distributed.) Observation error can be estimated by making κ replicate measurements of each unknown sample. Then,

$$\sigma_m^2 = \sigma_p^2 + \sigma^2(\epsilon)/\kappa \qquad (24)$$

$$\hat{\sigma}_p^2 = \sum_{i=1}^{n} (X_{i\cdot} - X_{\cdot\cdot})^2/(n-1)$$

$$\hat{\sigma}^2(\epsilon) = \sum_{i=1\&2}^{n} \sum_{j=1}^{\kappa}(X_{i,j} - X_{i\cdot})^2/[n(\kappa-1)]$$

where $X_{i\cdot} = \sum_{j=1}^{\kappa} X_{i,j}/\kappa$

$$X_{\cdot\cdot} = \sum_{i=1}^{n} \sum_{j=1}^{\kappa} X_{i,j}/(\kappa \cdot n)$$

and $f_1 = n - 1$

$f_2 = n(\kappa - 1)$

The approach of Gaylor and Hopper is illustrated in Table 3.

Variance correction methods have also been developed for the construction of tolerance limits for production quality control (Hahn, 1982; Mee, 1984; Jaech, 1984; and Mee, et al., 1986). The problem addressed is analogous to problems in water quality. It is desired to estimate the probability of a product failing specifications, but the probability estimate is based on measurements made with error. The crucial element is the desire to estimate the true probability of a product out of specification. In the context of water quality monitoring, the objective is detecting a violation of a standard, in contrast to estimating the probability of a measurement exceeding a standard. The distinction in the two objectives can be depicted with a normally distributed population sampled with observation error (Fig. 6). Figure 6 exaggerates differences between measurement and true distributions, but even small differences can cause a large difference in the coverage of a confidence interval (Porter and Ward, 1989).

The construction of tolerance intervals in the presence of measurement error is described by Jaech (1984), who considers criteria for using the SIDF method of estimating f for tolerance intervals. His criteria are similar to those of Gaylor and Hopper (1968). Mulrow et al. (1988) evaluated tolerance intervals using Satterthwaite's improved degrees of freedom when data were calibrated and found that they were conservative compared with nominal confidence levels. The opposite was true of confidence intervals from calibrated data.

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Table 3. Calculation of a SIDF confidence interval

This is an example of Satterthwaite's improved degrees of freedom. The process, X_p, is normally distributed with mean μ_p and variance σ_p^2 and $\hat{X}$ is normally distributed with mean μ_p and variance $\sigma_p^2 + \sigma^2(\varepsilon)$. The sample consists of 4 replicate measurements of four samples.

$$\hat{X} = \hat{X}_1 = 1.5 \quad 1.1 \quad 1.8 \quad 1.0 \qquad X_i. = 1.350 \qquad X.. = 1.988$$

$$\hat{X}_2 = 2.5 \quad 2.4 \quad 1.7 \quad 2.9 \qquad\qquad\quad 2.375$$

$$\hat{X}_3 = 2.0 \quad 1.7 \quad 2.9 \quad 2.2 \qquad\qquad\quad 2.200$$

$$\hat{X}_4 = 2.4 \quad 2.0 \quad 1.6 \quad 2.1 \qquad\qquad\quad 2.025$$

$$\hat{\sigma}^2(\varepsilon) = \Sigma\Sigma(X-X_i.)^2/[n(n-1)]$$

$$= (0.410 + 0.747 + 0.780 + 0.327)/12$$

$$= 0.189$$

$$\hat{\sigma}^2_m = \Sigma(X_i.-X..)^2/(n-1)$$

$$= 0.201$$

$$Q = 0.201/(0.189/4) = 4.261$$

$$f = (Q - 1)^2/[Q^2/f_1 + 1/f_2]$$

$$= (4.261-1)^2/(4.261^2/3 + 1/12)$$

$$= 1.733$$

A confidence interval is given by (for $\alpha = 0.05$):

$$CI = \hat{X} \pm t(1-\alpha/2,f)\hat{\sigma}_p S/(n)^{1/2}$$

$$= 1.988 \pm (5.00)(0.201 - 0.189/4)^{1/2}/2$$

$$= [1.008, 2.968]$$

$$f_M = \int_0^\infty f_{M/P} \cdot f_P \, dP$$
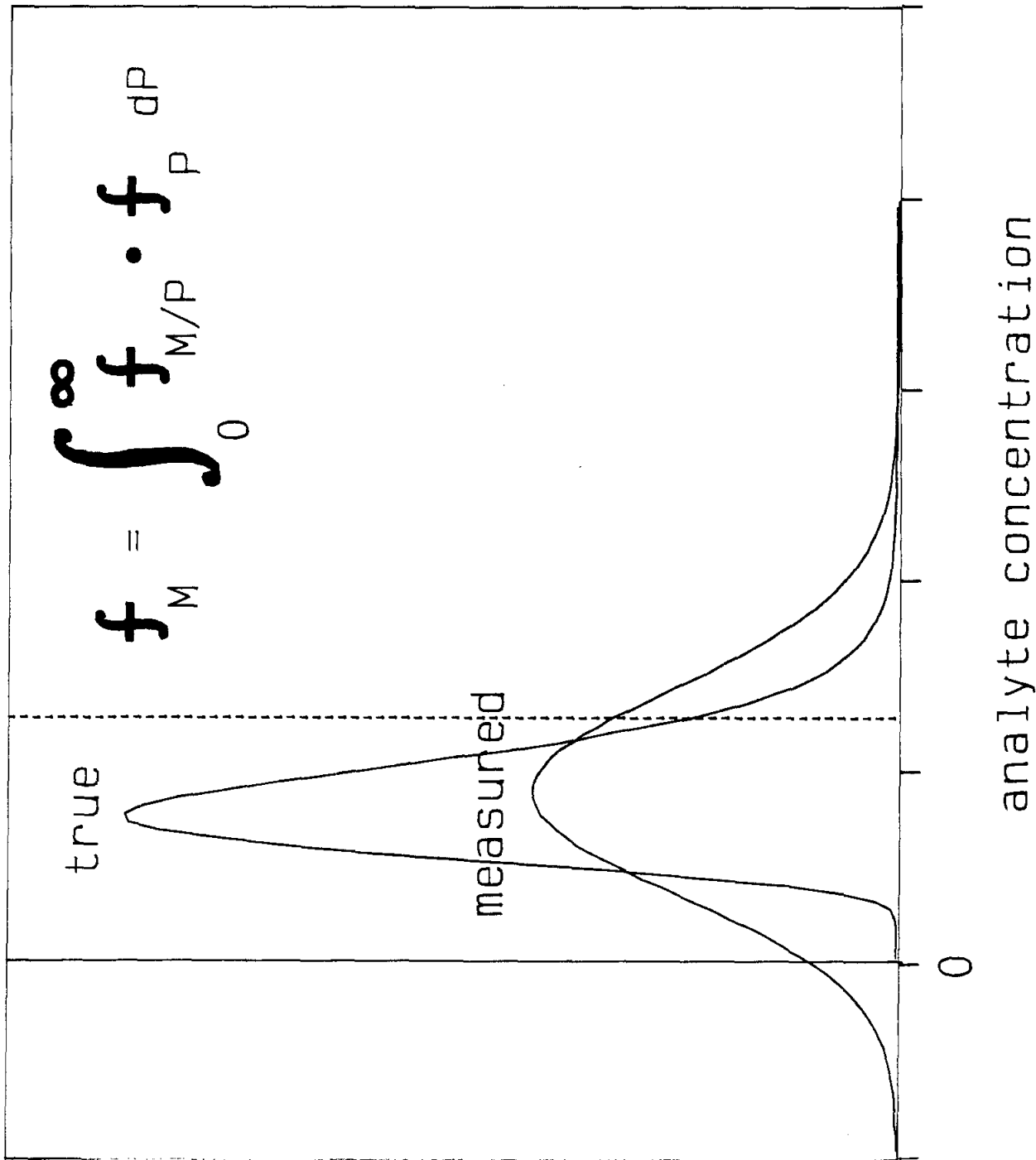
true

measured

analyte concentration

Figure 6. Convolution of a PDF by measurement

B. POE estimate of population variance

An important difference between variance correction applications in production quality control and water quality monitoring is the relative size of errors and the possibility of negative measurements. In production quality control, observation errors are usually small relative to variability in a manufacturing process. On the other hand, the relative error inherent in trace level water quality measurements is quite large. An estimate of the true process variance may be derived from equation (10), substituting sample estimates for true values:

$$\hat{\sigma}^2_p = [\hat{\sigma}^2_m - (r + s\bar{X}_p + t\bar{X}^2_p)]/(t+1) \quad (25)$$

Measurements were made of simulated samples from lognormally distributed population. The POE estimate was compared with the sample variance on the basis of relative efficiency (EFF) and root mean squared error (RMSE).

EFF = variance of estimate without error/
variance of measurements

RMSE = {Σ(parameter estimates - true
parameter values)²/
(number of simulations-1)}$^{1/2}$

The relative RMSE is the ratio of the RMSE for the POE estimate to the RMSE of the sample variance. The fraction of negative POE estimates was also calculated.

Calibration design, the coefficient of variation (CV) of the population, sample size, and the ratio LOD/ LOQ for the measurement system all had an impact on the performance of the variance estimate. The sample variance tended to be more efficient than the POE variance when LOD/LOQ was large (Fig. 7) but not when it was small (Fig. 8). Increasing the sample size or number of calibrants improved the relative efficiency of the sample variance when the LOD/LOQ was large, but again, not when it was small (Fig. 7).

The abscissa of Figs. 7-10 is the fraction of the population less than the LOD. As f_c increases, the POE estimate improves when LOD/LOQ is small (Fig.8) but not when it is large (Fig. 7).

Although the corrected variance estimator often has a larger variance than the sample variance, the relative RMSE shows that corrected variance is nearly always closer to the true process variance (Fig. 9). It may, therefore, be concluded that the corrected variance will lead to better confidence intervals for the population mean. An example of using the corrected variance to construct a confidence interval for the mean can be found in Table 4.

Even though corrected variance estimates are more accurate (lower RMSE) than uncorrected variance estimates, a large portion of these estimates are negative (Fig. 10). This presents a problem when constructing confidence intervals.

Consider Fig. 11, which illustrates the probability space of the various estimators of the mean and variance considered in this paper. The circles represent a region in which the true mean and variance lie with probability 1 - α. Observations made without error represent the smallest space. The space based on the sample mean and variance of measurements is larger and biased toward variance estimates which are too large because they include measurement variability. The region based on corrected variance estimates is smaller than the region based on measurements, but includes negative mean and variance. Estimators, which occupy a probability region and which excludes areas of negative mean and variance estimates, would be the best. Further work is needed to develop a confidence interval based on a reduced probability space.

V. Summary

Trace level measurements are characterized by a lack of precision. Information derived from such measurements is not useful unless the component of random variability is properly interpreted. In the past, it has been
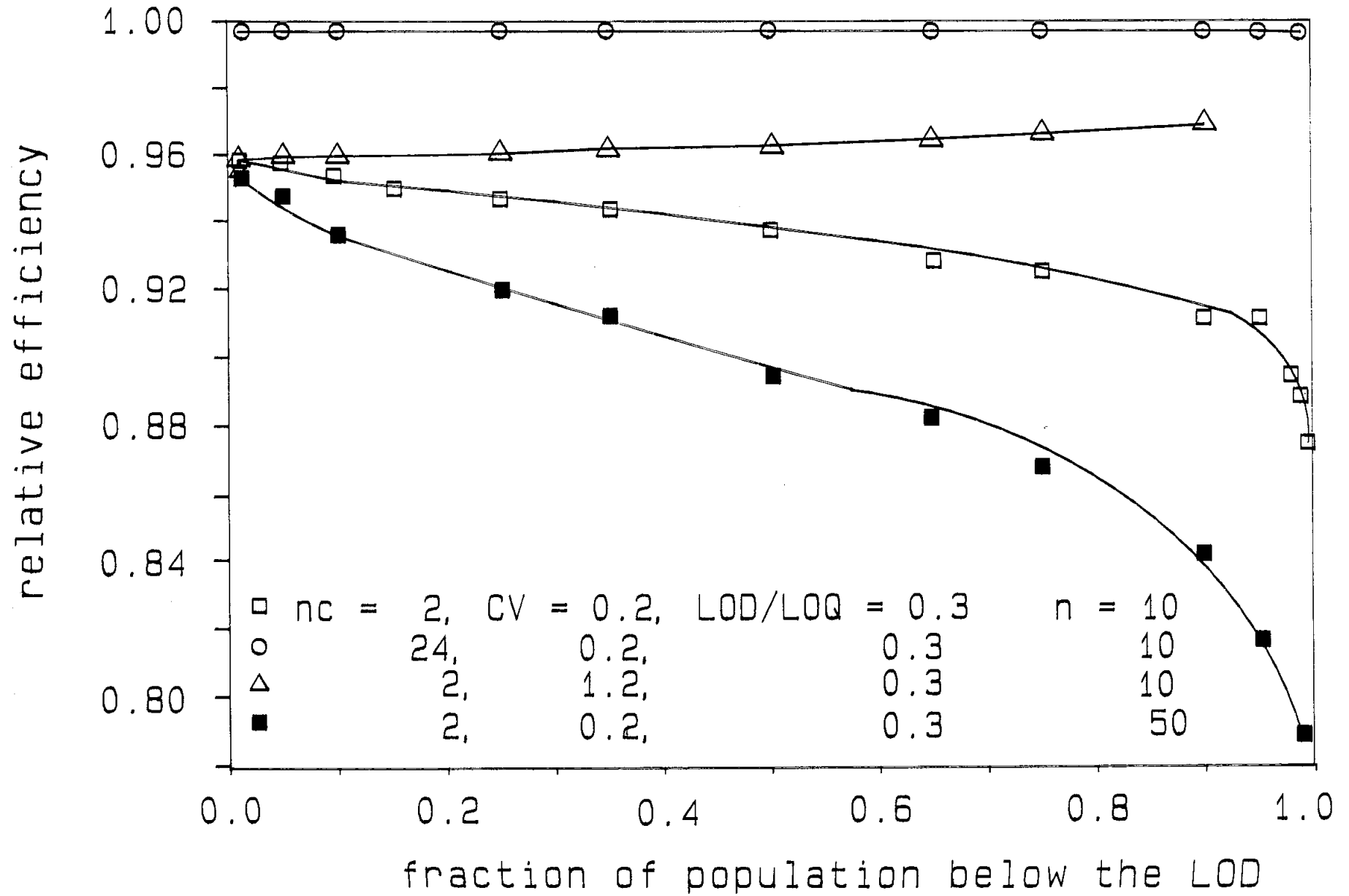
Figure 7. Efficiency of corrected variance estimate relative to
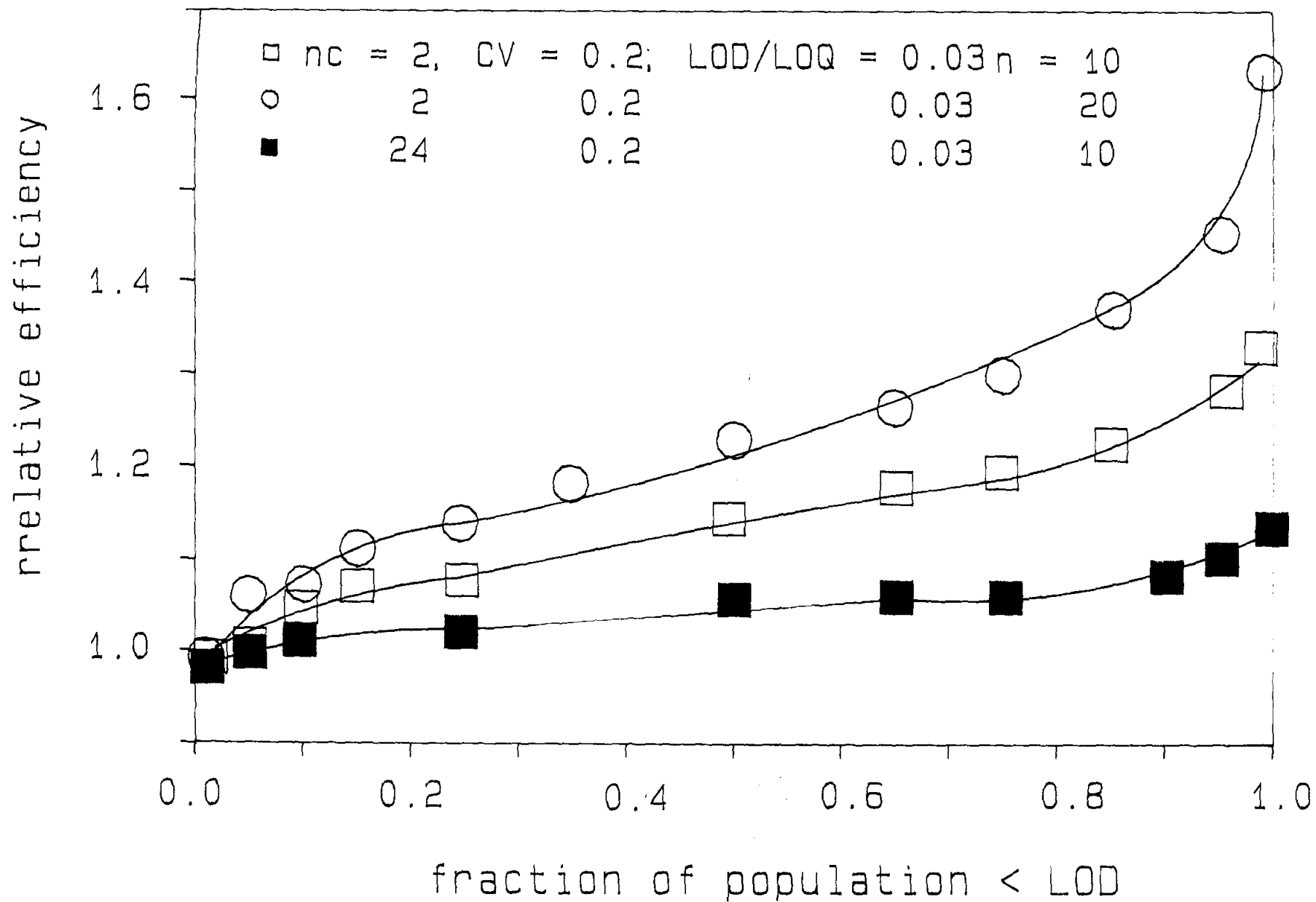
Figure 8.   Efficiency of corrected variance estimate relative to
            sample variance when R = 0.03

□	nc	=	2,	CV	=	0.2,	LOD/LOQ	=	0.3	n	=	10
○			24,			0.2,			0.3	n	=	10
△			2,			1.2,			0.3	n	=	10
●			2,			0.2,			0.03	n	=	10
■			2,			0.2,			0.03	n	=	20
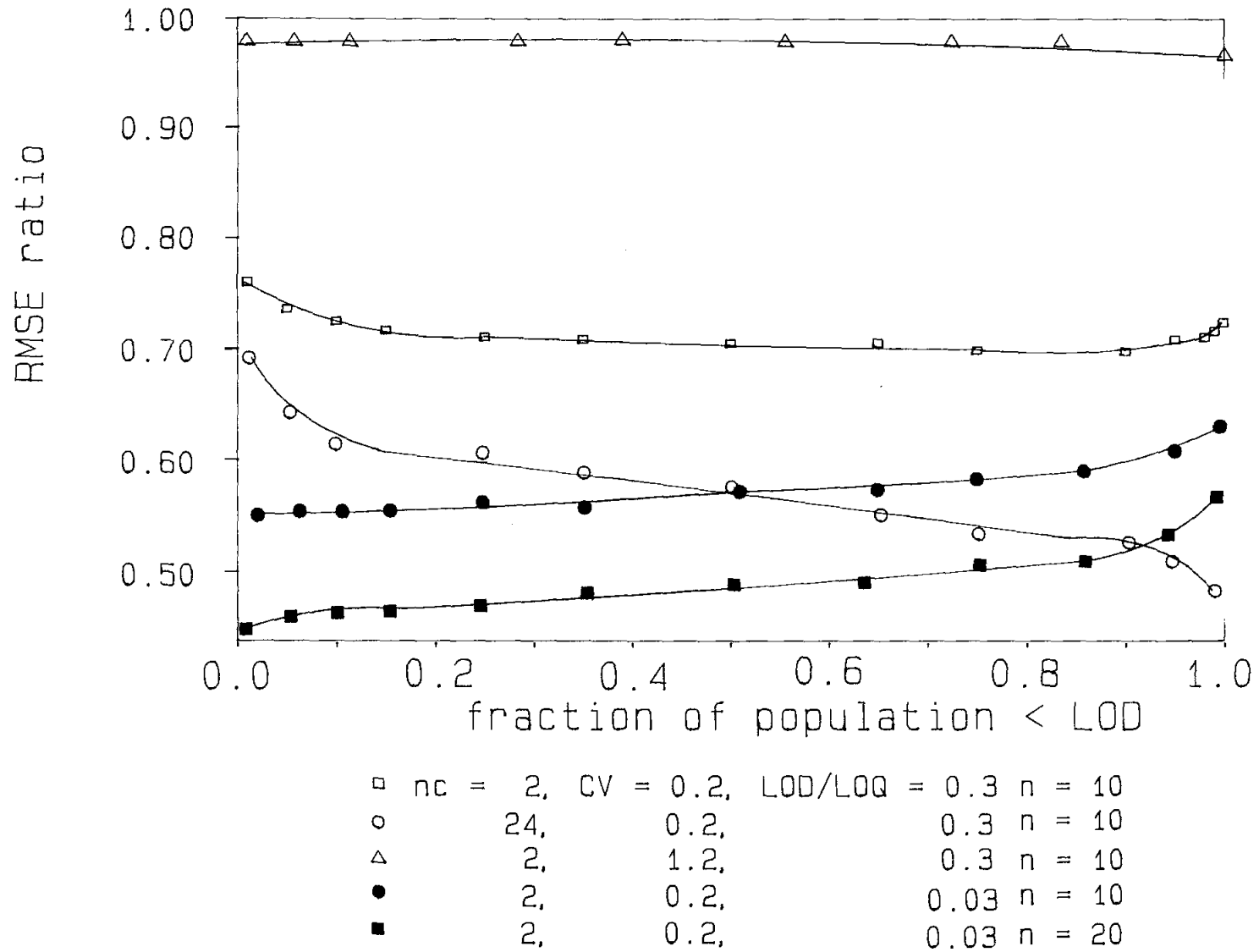
Figure 9.   RMSE of corrected variance estimate relative to
             sample variance

Table 4. Calculation of a corrected variance confidence
interval

Laboratory experiments have found the following to be true:

LOD   = 1.0

LOQ   = 20.0

LOD/LOQ = 0.05

k_0 = 0.111

k_1 = 0.194

A two point calibration with X = 0 and X = 5 was used for each

measurement. On the basis of weighted least squares and

equation 5:

$\sigma^2(b_0)$ = 0.111

$\sigma^2(b_0, b_1)$ = -0.022

$\sigma^2(b_1)$ = 0.0058

r = 0.222

s = 0.172

t = 0.0058

$\hat{\beta}^2$ = 0.545

confidence interval = [0.308 0.946]

Some improvement this time.

Figure 10. Fraction of corrected variance estimates which are negative

Probability Space

possible space of underlying process

Figure 11. Probability space of mean and variance estimates.

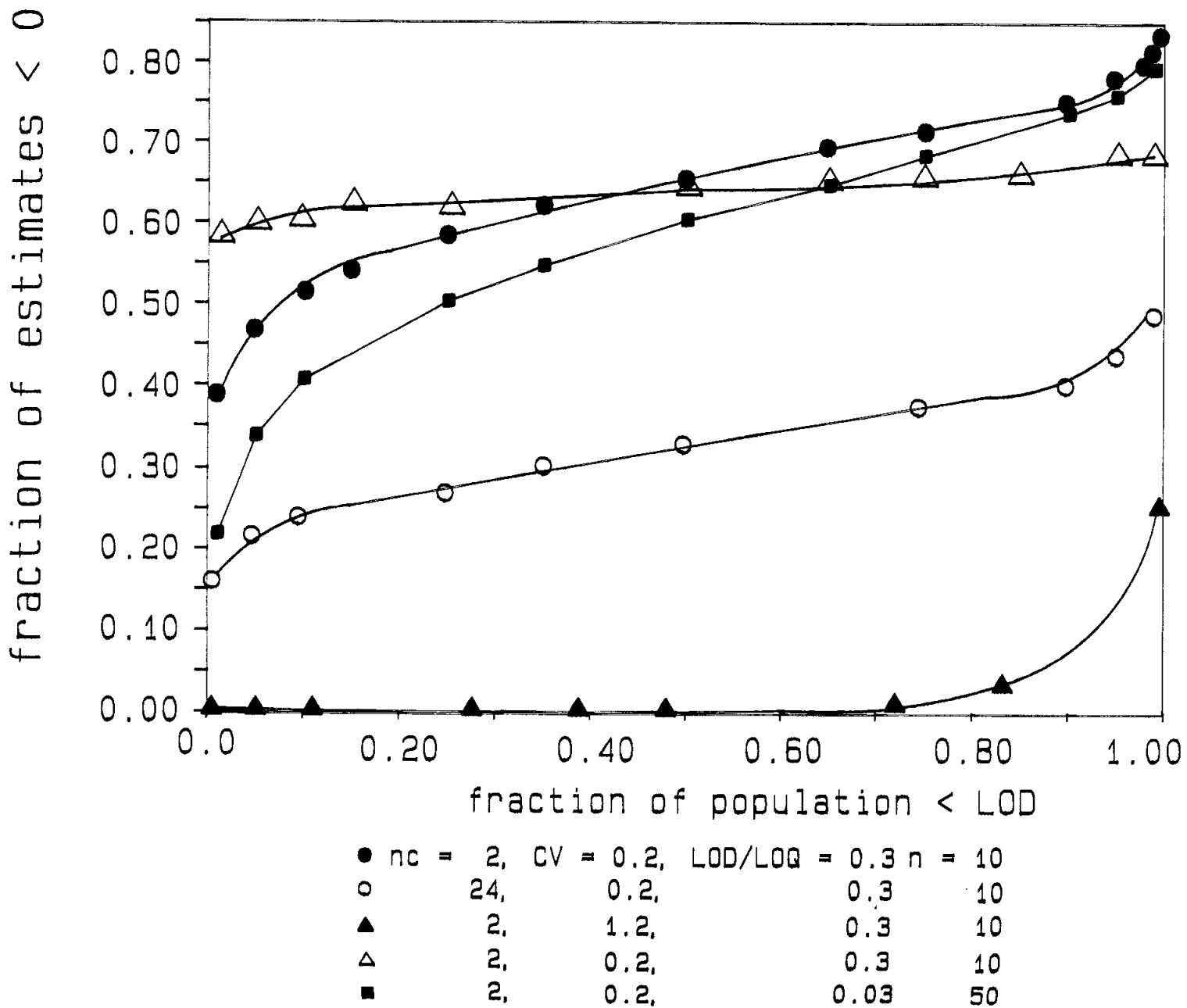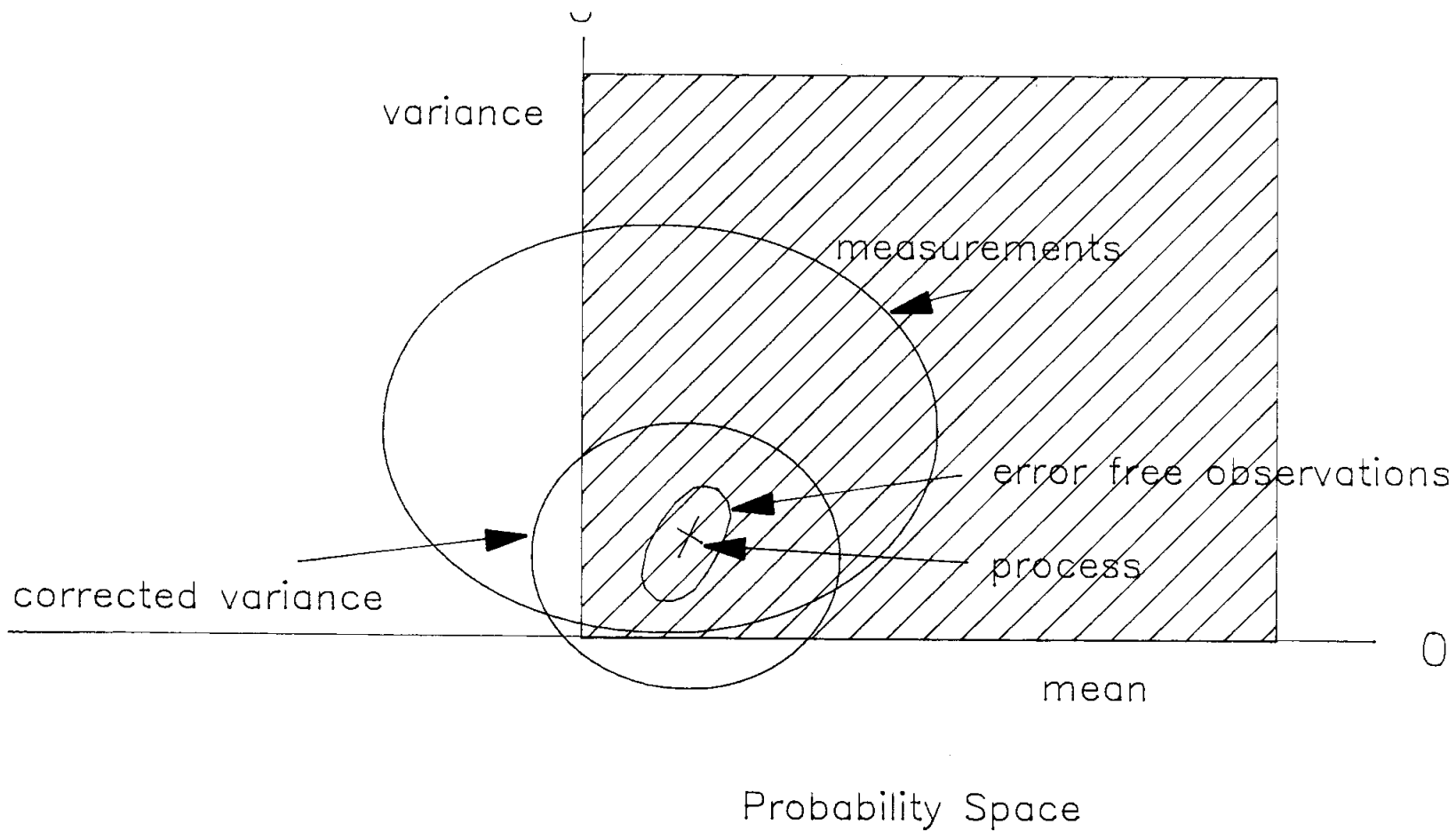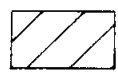the analyst who enforced standards of data quality related to detection by censoring data according to criteria based on random signal variability. However, censoring (results of ND or LT) results in a loss of information. In addition, methods for censored data are less familiar and more complicated than those for uncensored data.

Uncensored data permit the use of statistical methods which are familiar to non-statisticians. Classical statistics based on the normal distribution will often be appropriate because random measurement error is often normally distributed. Distributions of measurements are more symmetric than skewed processes. Distribution free methods, used when data are not normally distributed, are also easier to apply when data are not censored.

Information derived from measurements, censored or uncensored, may not shed much light on a process unless measurement variability is segregated from process variability. When constructing a confidence interval for the mean of a population, a Bayesian t statistic or corrected variance technique may be useful. Conditioning Student's t statistic on the basis of a positive true mean will eliminate confidence intervals which overlap 0 and will be smaller than unadjusted confidence intervals. Solubility considerations may further reduce the range of possible statistical outcomes.

Variance correction methods, in theory, improve statistical analysis of trace level measurements. In practice, negative variance estimates will often occur. The problem of negative variance estimates can be made more tractable by contrasting the probability space of variance and mean estimates with acceptable outcomes (positive true mean and variance).

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LABORATORY INFORMATION MANAGEMENT: AN INTEGRAL PART OF WATER QUALITY MONITORING SYSTEMS.

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1. INTRODUCTION

1.1 Background

The mission of the Republic of South Africa's Department of Water Affairs with respect to water quality management is to ensure that water of an acceptable quality for recognized water uses, such as urban, industrial, agricultural, recreational and environmental conservation uses, continues to be available (Department of Water Affairs, 1986). Within this mission, the role of the Hydrological Research Institute in water quality assessment is to provide the information that will assist water quality managers in making sound decisions.

Until recently the Department of Water Affairs operated three major water quality monitoring programmes. Two of these were aimed at the assessment of the quality of South Africa's surface and groundwater resources. The third was designed to provide information on the quality of effluents and is primarily used for regulatory purposes. Data collected in these programmes were frequently found to be inadequate, not in the sense of there not being enough, but in terms of setting objectives, for formulating alternative water quality management strategies, for making decisions, and for evaluating results against planned objectives. In response to these changing demands for information - information that is essential to the assessment of water quality management actions - two of these monitoring programmes are currently being redesigned according to procedures recommended by Ward (1988). The first of these is a national monitoring system that will provide information on the existing water quality conditions in the country and how the quality is changing. The second monitoring system is a regional or catchment specific monitoring system which differs from the national programme in both level of focus and detail. The focus of this programme will be on the identification of areas and causes of water quality problems and to evaluate and predict the effect of water quality management actions.

As a direct result of these revised monitoring structures, the need was also recognized for a cohesive laboratory information management system to provide for the centralized control of information concerning water quality monitoring networks and related clients, samples and results in the Department's analytical laboratories located at the Hydrological Research Institute.

1.2 Analytical Service Laboratories

The Hydrological Research Institute's analytical service laboratories are the primary source within the Department of reliable qualitative and quantitative information about any sample and its chemical and/or biological constituent composition.

Analyses are performed within a four laboratory organizational structure. The four functional laboratory groups are; a laboratory which primarily utilizes state-of-the-art automation for major ion and nutrient analyses, a spectroscopy laboratory for metal analyses, a chromatography laboratory responsible for organic residual analysis and characterization and a biology and bacteriology laboratory. The total workload of these groups is approximately 35000 samples per year for an estimated 300000 to 400000 individual tests. Major analytical equipment includes a number of inductively coupled plasma and atomic absorption spectrometers, gas/liquid and liquid/liquid chromatographs, AutoAnalyzers and a mass spectrometer. The samples received at the laboratories are primarily water, but a significant number of fish, soil, sediment and solid wastes samples are also included.

1.3 Laboratory Information Management

The overall motivation for automation and the management of information in analytical laboratories is to enhance the quality of laboratory data, improve the laboratory productivity (i.e. cost reduction) and more importantly provide water quality management with more timely and reliable access to water quality data. However, to satisfy these objectives the development should be approached from the viewpoint of the management of information as opposed to the more conventional strategy of computer hardware and software development.

For the purpose of this paper, a Laboratory Information Management System (LIMS) is defined as follows: a systematic, formal federation of subsystems that perform data management and chemical analysis operations to (a) meet transactional data processing requirements in the laboratory, (b) provide information to the laboratory management in support of controlling and planning activities, and (c) provide data as an input for a later processing cycle, e.g., the storage and analysis of water quality data.

A Laboratory Information Management System (LIMS) is therefore an assemblage of interlinked subsystems, each of which has unique functional responsibility. These functional subsystems include, at the heart of the LIMS, a Sample Management System (SMS) and, depending on the laboratory structure and functions, one or more subsystems generally referred to as an Instrument Automation System (IAS) or Instrument Management System (IMS). Figure 1 is a schematic diagram of the LIMS configuration, showing the various components of the system developed in the Institute's laboratories.

This paper discusses the approach that was adopted by us in the design of the Sample Management Subsystem of the LIMS. In addition, it provides an overview of the system developed for the Institute's analytical service laboratories to, (a) maintain and track sample information related to specific water quality monitoring programmes and projects, (b) to provide integrated quality management, (c) to provide an automated interface to the remotely located National Water Quality Database, and (d) to provide automated interfaces to a number of Instrument Automation Subsystems.

2. SYSTEMS DESIGN APPROACH

2.1 Introduction

Systems design can be defined as the process of planning and structuring of the many separate components of a system into a practical integrated whole and is primarily concerned with the development of specifications for a proposed new system.

The development of Laboratory Information Management Systems often proceed at an inconsistent rate and with limited success because of a number of factors, such as lack of experience, inadequate programming support and more importantly the absence of an adequately structured system specification and design approach.

The design of a SMS is a complex problem, and should be solved by a systematic and creative approach. For this purpose, the SMS design should be separated into a number of well defined tasks, which are executed in a
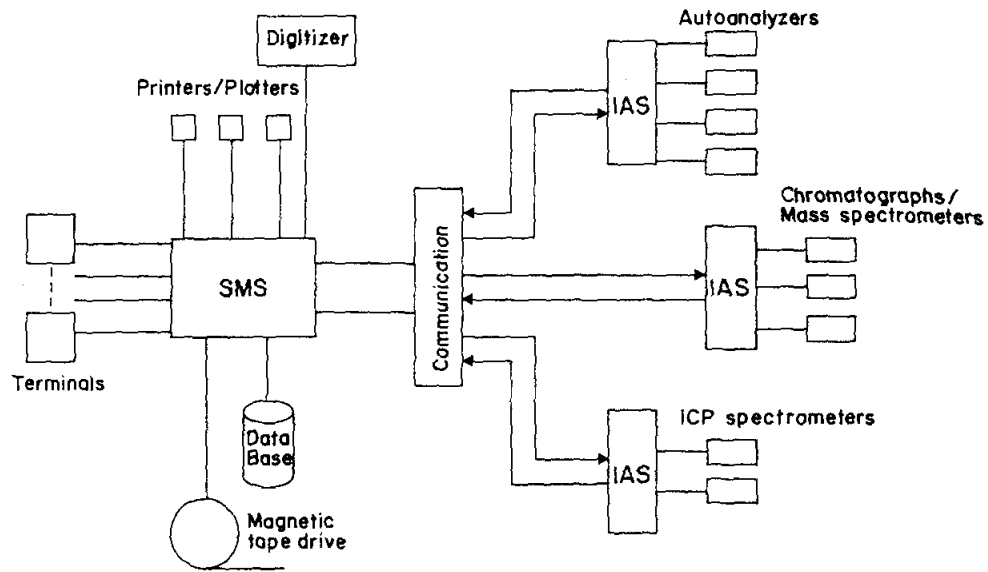
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Figure 1: Schematic diagram of the LIMS configuration, illustrating the various components of the total system.
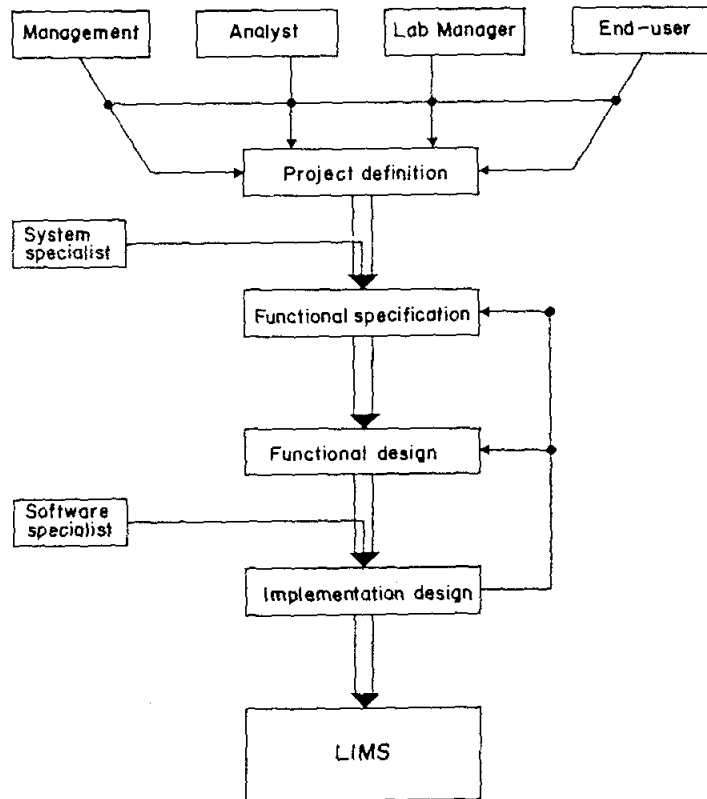

Figure 2: Outline of a structured procedure in which thephases of a system design process are illustrated.

logical sequence. These tasks include: project definition, *system specifications, functional design* and implementation. The first three tasks can and should be completed without considering hardware, propriety software or database specifications. The subsequent implementation can then proceed with a minimum uncertainty to provide a system that will meet the information requirements.

An outline of a structured procedure is shown in Figure 2, in which the aspects of project definition, system specifications, functional design and implementation are illustrated. Although Figure 2 indicates that the design procedure is executed as separate tasks, it should be understood that numerous iterations are usually required between system designer, software developers and the laboratory manager and staff to develop the system. From the start, the development should be documented and where possible systems evaluation criteria should be established for the final implementation stages.

The aim of this brief discussion presented here is to illustrate the framework which served as a basis for the structured design of our system.

2.1.1 Project definition

The primary purpose of the system definition is to force all parties to formulate a mutually agreed upon definition of the requirements of the system. In essence the definition becomes a statement of the overall objectives. Clearly, the basic informational requirements should be extensively investigated and should come from several sources, including water quality management (the end-user) and the laboratory management and staff. To illustrate this step, some general goals of a SMS project can be summarized as follows:

1. Accept and maintain information related to water quality monitoring programmes, establish and maintain links between samples, sampling locations and the associated water quality variables to be measured and clients.

2. Accept test results from various laboratory sources and field measurements. The system must support single result as well as multiple (fixed and variable number) result analytical procedures. In addition, the data base must be capable of storing results in either text or numeric form.

3. Provide laboratory staff with functions to edit and update previously entered data.

4. Provide laboratory management and staff a range of interim and final reports, such as backlog, test result and quality management reports.

5. Provide integrated analytical quality management and error checking throughout the data processing cycle to minimize errors in manually entered data where possible.

6. Provide laboratory staff with functions to accept or reject analytical results on a *sample or individual result basis.*

7. Provide functions to selectively archive data from the SMS data base.

8. Provide functions to selectively retrieve data from archive into separate databases.

9. Provide a link to a remotely located National Water Quality Data Base for the transfer of completed sample results on the basis of selected water quality monitoring projects.

2.1.2 Functional specifications

One of the most important documents to prepare contains the system specifications. This phase of the process answers the questions of what the present system is doing, and more importantly what is to be accomplished to meet the requirements of the system and not how it should be done.

The problem of developing the system specifications is primarily one of definition of

terms. That is, if the requirements of the SMS are sufficiently well defined, the procedures to generate the specifications are greatly simplified. However, at this stage of the design process the participation of the systems specialist becomes essential.

Within each major functional section of the SMS (Figure 3), the functions related to it can be subdivided into two categories; (1) system maintenance (update/edit functions) and (2) data retrieval (archiving and report generation functions). To serve as an example, the functional specification of an Edit function is given here.

ANALYSIS RESULT EDIT - The user must be provide with a function to edit the results of analyses which have been entered into the system either manually or via an IAS. The user must be able to identify the sample to be edited by entering the SAMPLE ID or the WORKSHEET ID and WORKSHEET POSITION. Alternatively, by selecting the WORKSHEET ID the user must be allowed to step through the samples in the worksheet to find the one to be edited. The user must be allowed to update selected fields from the ANALYSIS RESULT TABLE but must not be allowed to insert new records or delete existing records. The function must automatically set the RESULT STATUS to "complete". No editing must be allowed on results which have already been approved. The following fields must be used to access the sample to be edited:

- SAMPLE ID- unique sample identification assigned by the SMS

- WORKSHEET ID- unique worksheet identification generated by the SMS

- TEST CODE- code referring to analytical method defined in analysis protocol table

2.1.3 Functional design

Upon completion of the specifications, a functional design should be developed. In contrast to the specification phase, the functional design phase is concerned with how

the system will meet the requirements. Functional designs are detailed descriptions and graphical representations of each function. It therefore includes all the functions related to the various sources of data (input screen layouts), the interconnecting processing requirements, the data base file structures, and outputs (e.g. type and layouts of report). It is a detailed blueprint which allows the software development group to generate the code to transform the design into hardware and software for the implementation.

Once the functional design phase is commenced, invariably new questions will arise regarding the specifications. Similarly, once the functional design is complete, and the implementation stage is reached, an iteration back to the specification and functional design phase, in order to correct and adjust the design, may be necessary. The strategy to converge most constructively on a good design is to follow some structured approach, and have as many iterations between the various phases as required.

3. SYSTEM OVERVIEW

3.1 Introduction

The main rationale for a sample management system is to track samples and process the data produced on these samples from the time they are received in the laboratories, through the analyses and quality assurance of results, to some form of the final reporting. At the most elementary level our laboratories receive samples from a number of water quality monitoring networks, analyze them and transfer results to the National Water Quality Database. The flow of samples and related information through the SMS is illustrated in Figure 3.

Four major functional areas of the SMS can therefore be identified. These are, (a) input of sample information, (b) results entry and edit, (c) quality assurance and approval of samples, and (d) archiving and transfer of sample information to the National Water Quality Database. Each of these functional areas of the SMS is supported by a number of functions (Table 1). However, a detailed
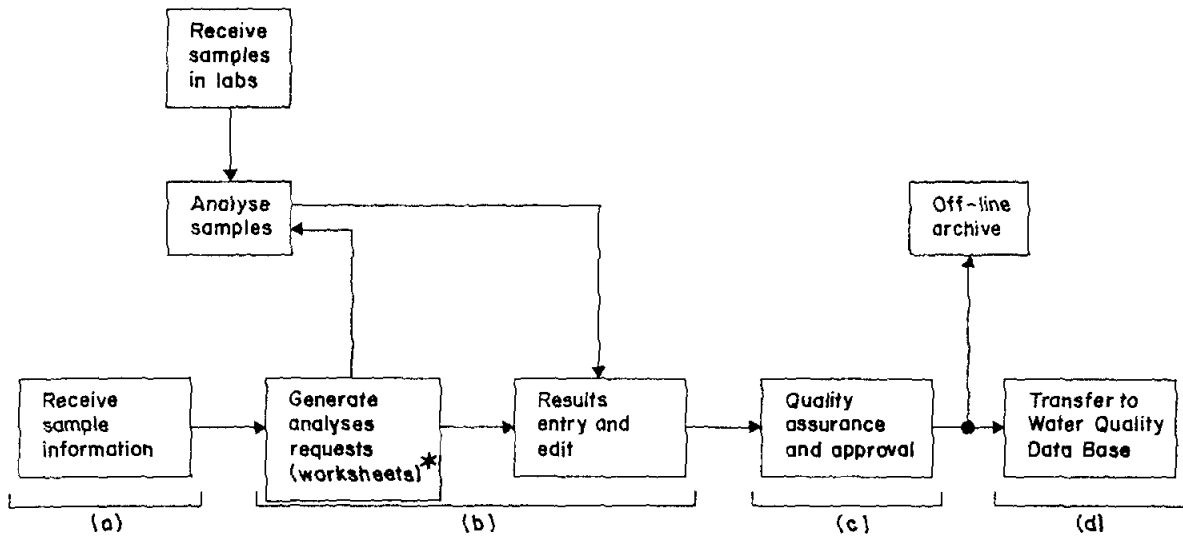
Figure 3: Flow of samples and related information through the SMS. (a) Sample information entry/edit, (b) Result entry/edit, (c) Sample approval, and (d) Archiving and transfer to database.

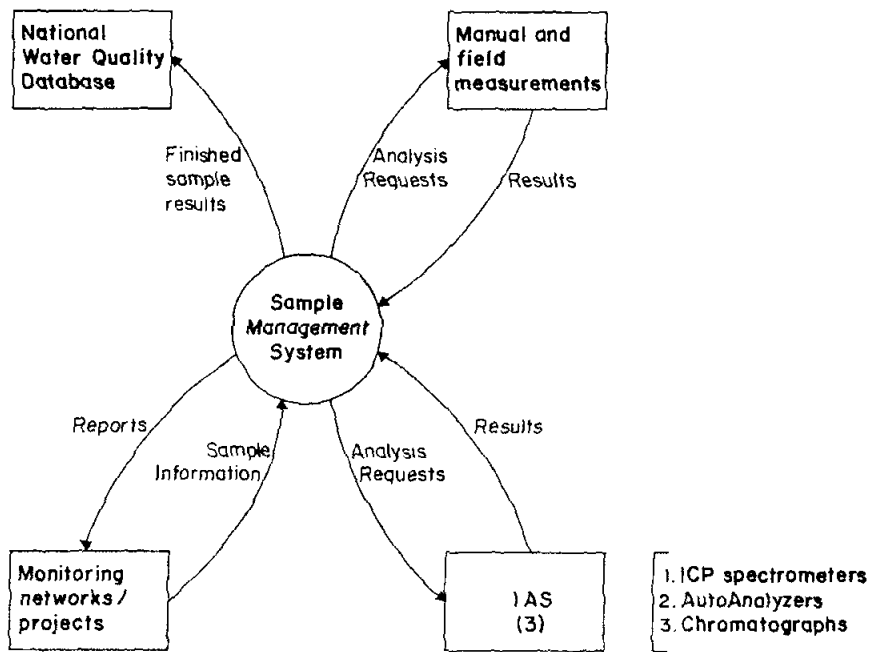Figure 4: A context diagram of the SMS showing the various interactions between the system and the outside world.

TABLE 1:   Selected menus and related functions of the Sample
             Management System.

             MENU   FUNCTIONS
----
1 - ADMINISTRATIVE MENU   Client entry/edit
                                   Project entry/edit
                                   Sample source entry/edit
                                   Analysis entry/edit
                                   Analysis group entry/edit
                                   Project vs Source entry/edit

3 - SAMPLE PROCESSING MENU   Sample login - by sample
                                   Sample login - by batch
                                   Sample information edit
                                   Cancel sample
                                   Cancel sample in worksheet

5 - RESULTS PROCESSING MENU   Analysis result entry - by
                                   sample
                                   Analysis result entry - by
                                   worksheet
                                   Edit analysis request - by
                                   sample
                                   Cancel analysis request - by
                                   sample
                                   Analysis result edit
                                   Quality control

6 - REPORT MENU   Database tables report
                                   Lookup list reports
                                   Result reports
                                   Backlog report
                                   Quality control report
                                   Sample information report
                                   Worksheet report
                                   Sample progress report
                                   Trend display
                                   Project report
                                   Source report
                                   Source vs Project report

discussion of each of these functions is beyond the scope of this paper, only the system interface requirements are discussed.

3.2 System Interface Requirements

The term system interface refers to those segments of the SMS which interact with the outside world. In the following sections the interaction of the SMS with IA subsystems, the national water quality database, water quality monitoring networks and projects, and the laboratory staff, are discussed.

Figure 4 is a context diagram of the SMS showing the various interactions between the system and the outside world. As illustrated in the diagram there is one external user of the SMS information, i.e., the National Water Quality Data Base. Similarly, two sources of data are the monitoring networks producing sample information and the laboratories providing the analytical results. The latter sources consists of three Instrument Automation Subsystems utilized in the laboratories for, (1) major ion and nutrient analyses, (2) trace metal analyses, (3) organic residue analyses and characterizations and the manual and field measurement procedures.

3.2.1 Instrument Automation Systems

A major consideration in the development of our SMS was to establish functions which automated the input to the system of test results originating from various sources (instruments and procedures) in the laboratories. The objective was to transfer as many as possible of the analysis results generated in a laboratory to the SMS via electronic links established between the SMS and its subsystems; an approach which also eliminated the need for error-prone manual transcription and entry results. This is certainly of significant benefit to the laboratory staff working with automated instruments and other high volume computerized laboratory equipment, particularly in view of the large number of analyses routinely carried out by these procedures in a single day.

Analytical procedures and the related equipment in water laboratories can be divided into three basic groups:

The first group of instruments, used extensively in water laboratories, are those based on the continuous flow analysis principle (e.g. AutoAnalyzers). These instruments are, in general not computerized (or so-called software-driven equipment) and many laboratories have undertaken the in-house development of Instrument Automation Systems. These systems primarily focused on instrument-control, on-line, real-time data-acquisition, quality control and data reduction. As part of our LIMS development, the implementation of this IAS was undertaken in parallel with the SMS development.

The second group of instruments are those devices which utilize computers as an integrated part of the equipment and can consequently be treated in the SMS as IA Subsystems. Unfortunately, the computer compatible data-communication facilities which are normally incorporated in the equipment, operate at different levels of intelligence. This lack of a standard data communication protocol for analytical equipment can be a major obstacle, and dictates that each subsystem must be treated as a unique interface to the SMS.

For both types of subsystems, data communication between the SMS, and IA Systems, was established as tasks that are executed in the background, completely transparent to the laboratory staff. The laboratory staff is provided with a function on the SMS to generate worksheets which consist of samples sorted according to a particular group of variables (required analysis). Once a worksheet contains the required number of samples, it is automatically transmitted to the IAS responsible for the particular group of analyses. On completion of the analyses and quality assurance, the completed worksheet and associated results are automatically returned to the SMS. This in turn initiates a function in the SMS to update the relevant fields in the database.

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The third group consist of those methods and instruments used manually in the laboratory or in field measurements. Although not part of the instrument interface, worksheets are also generated by the SMS, but downloaded to printers located in the laboratory responsible for those particular manual analysis. Through the user-interface (section 3.2.4), a function is then available to the laboratory staff to update the SMS database.

3.2.2 National Water Quality Data Base

Analytical results, prior to being released to a client, must be approved by authorised laboratory staff. Once the samples related to a particular water quality monitoring project have been approved, the final results are formatted into the required data records and stored in a transaction file. These files are then automatically transmitted, via a network, to the national water quality data base. In addition to the nation wide monitoring programmes, samples related to completed research or surveillance projects are stored on archive files (magnetic tapes) and then deleted from the SMS database. These files primarily serve as backup, but facilities have also been created to retrieve these sample results to a separate database.

3.2.3 Water quality monitoring networks

In terms of the SMS, a project is defined as any monitoring activity that will generate and submit samples for analyses to the laboratories. The design document or project proposals, is required to record the sampling locations (sample sources), sample dates/ frequencies, as well as the required analyses to be performed per source and sample type, in the SMS. Within the SMS database, a unique relationship is then established between the project, its sample sources and related required analyses. The idea of this is to provide the laboratory staff with a way in which to enter samples and required analyses into the system as compactly and efficiently as possible at the project/source level. Consequently, during a sample login session, only the: (1) project id., (2) source id., (3) sample type, and (4) date/time sampled are required to uniquely identify the sample and

analyses to be performed, in the SMS. In addition, by employing the information on the PROJECT and SOURCE TABLES, it is possible to generate, for example sample collection lists and laboratory workload projections.

3.2.4 User interface

The SMS is a menu-based system which allows the laboratory staff to communicate with the system by selecting options from menus displayed on terminals. Throughout the system all functions associated with the entry, editing and processing of data and sample information is available to the laboratory staff through this tree-structured menu system. A summary of selected menus and related functions, grouped together according to their use in the laboratories, is given in Table 1.

Wherever possible, data input to the LIMS is checked for validity during the actual input, edit or update activity. An extensive array of lookup tables serve as the references against which the data entries are validated.

4. CONCLUSIONS

The purpose of this paper has been to discuss only some of the many aspects of the development of a laboratory information management systems. Clearly, all these systems call for some kind of computer configuration and application software development, necessary to meet the systems requirements. Justification of any proposed computer configuration, or any other aspect of the system requiring capital and time investment, should be stated in terms of a cost/effectiveness analysis. This approach weighs the direct and indirect benefits derived of a proposed system against resource limitations such as cost. Such an analysis is a critical requirement of any system development and determines if the proposed system produces benefits which outweigh cost.

The decision to develop a system from scratch, or whether an acceptable system is commercially available is not new to the management process. However, the choice

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between making or buying, very often represents a critical decision of which the laboratory management must be aware. Based on our experience with the development of our LIMS, the advantages of, (1) a system tailored to requirements, (2) a high degree of integration into the water quality information system, (3) the optimum use of our organizational resources, and (4) the utilization of advanced state of the art techniques, more than outweighed the disadvantages of the additional cost and relatively long development time.

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WATER QUALITY INFORMATION MANAGEMENT SYSTEM

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1.0 Introduction

Technical Information Management Systems (TIMS) has been developed at WESTON for years. WESTON TIMS was initiated to develop problem solving computerized methodologies and software for application to meet the environmental objective of conducting site-oriented, multidisciplinary characterization and analysis. The major focus and strengths of WESTON TIMS are information management and site characterization. WESTON recognizes the importance of enhancement of TIMS analytical and modeling capabilities. This paper describes the efforts of developing water quality information management and its use in a water quality modeling system.

The water quality model used in this paper (DIURNAL) was originally developed at Manhattan College and was modified by the Environmental Protection Agency Region III and WESTON into its present form.

The concentration of dissolved oxygen (D.O.) is an important factor in the evaluation of water pollution and in the management of water quality. The diurnal water quality modeling is a modeling technique to predict D.O. of stream water through the proper evaluation of photosynthesis and respiration rates of aquatic plant communities.

The purposes of this research is:

- To develop a PC-based, water quality information system,

- To combine information management, information display and water quality modeling into one integrated system,

- To provide a menu-driven ready-to-use system which requires of the users minimum knowledge of computer languages.

2.0 System Specification and Requirements

This section describes the system specification which involves the formalization of system requirements, including software and hardware requirements and the statements of system functionality.

2.1 System Requirements

The system is required to be a user-friendly menu-driven system which can be implemented on IBM PC or compatible. The system integrates the capabilities of data entry, database management, reporting, analysis, graphics and water quality modeling together. User's knowledge of computer languages should be kept to a minimum and on-line help facilities should be available. The system should have the flexibility of modifying existing modules or adding new modules in the future.

2.1.1 Software Requirements

The important considerations for the system host language are database management, modeling capabilities, reporting and graphical capabilities. The commercial software package available on the market that meets these requirements and needs is SAS Institutes' PC-SAS[1] Version 6.03 which runs under DOS version 3.0 or later version. The PC-SAS[1] products are discussed as follows:

- Base SAS[1] - for data retrieval and management, programming, statistical, and reporting capabilities,

- SAS/AF[1] - for full screen, interactive front end to other SAS applications,

- SAS/FSP[1] - for interactive menu-driven editing, data entry, data retrieval and message processing,

- SAS/STAT[1] - for regression analysis, multivariate analysis, and other advanced statistical procedures.

- SAS/GRAPH[1] - for high - resolution graphics.

2.1.2 Hardware Requirements

The hardware configurations in which the PC-SAS and application program will reside are as follows:

- Computer - IBM[2] PC or compatible,

- Minimum memory - 640 Kbytes RAM with 4 Mbytes expanded memory,

- Minimum disk configuration - a hard disk with 20 Mbytes memory,

- Output device - printer or plotter are optional.

3.0 System Implementation and Design

After successfully entering the system, the user will see the MAIN MENU selection screen. This menu enables the user to navigate through the system. The system consists of five functional modules. The system functionality flowchart is shown in Figure 1. A detailed discussion of each module follows.

3.1 Data Entry/Maintenance Module

This module allows the user to access menus from which a particular type of data can be added, deleted, updated or reviewed.

The data entry screen selection includes:

- Facility information

- Location information

- Ground water level data

- Water quality analytical tests

- Water quality data information

- Parameter definition information.

The water quality data selection consists of:

- Sample station information

- Diurnal dissolved oxygen sample point data

- Laboratory data (with NBOD)

- Laboratory data (without NBOD).

The water quality data from the project of "Wasteload analysis of the receiving stream for the city of Huntsville" was utilized for this protocol development. The study area is located in Madison County in northwest Arkansas. Treated wastewater from the Huntsville wastewater treatment plant is discharged into Town Branch which flows into Holman Creek and ultimately to War Eagle Creek. An intensive stream sampling survey was conducted on Town Branch, Holman Creek, and War Eagle Creek as well as the Huntsville wastewater treatment plant effluent. This study area included eight stream sampling locations.

Using SAS/FSP software to create data entry screens, we can facilitate methods for performing interactive, full-screen facilities for data entry, editing, and data retrieval; and for interfacing with internal data files.

The fill-in-the-blank type of data entry screens, which closely resemble the formats of data collection forms, make the data entry job much easier. Data is simply entered into the system through the corresponding data entry screens. The Base SAS software manages system data files and serves as database manager.

FIGURE 1   FUNCTIONALITY FLOW CHART

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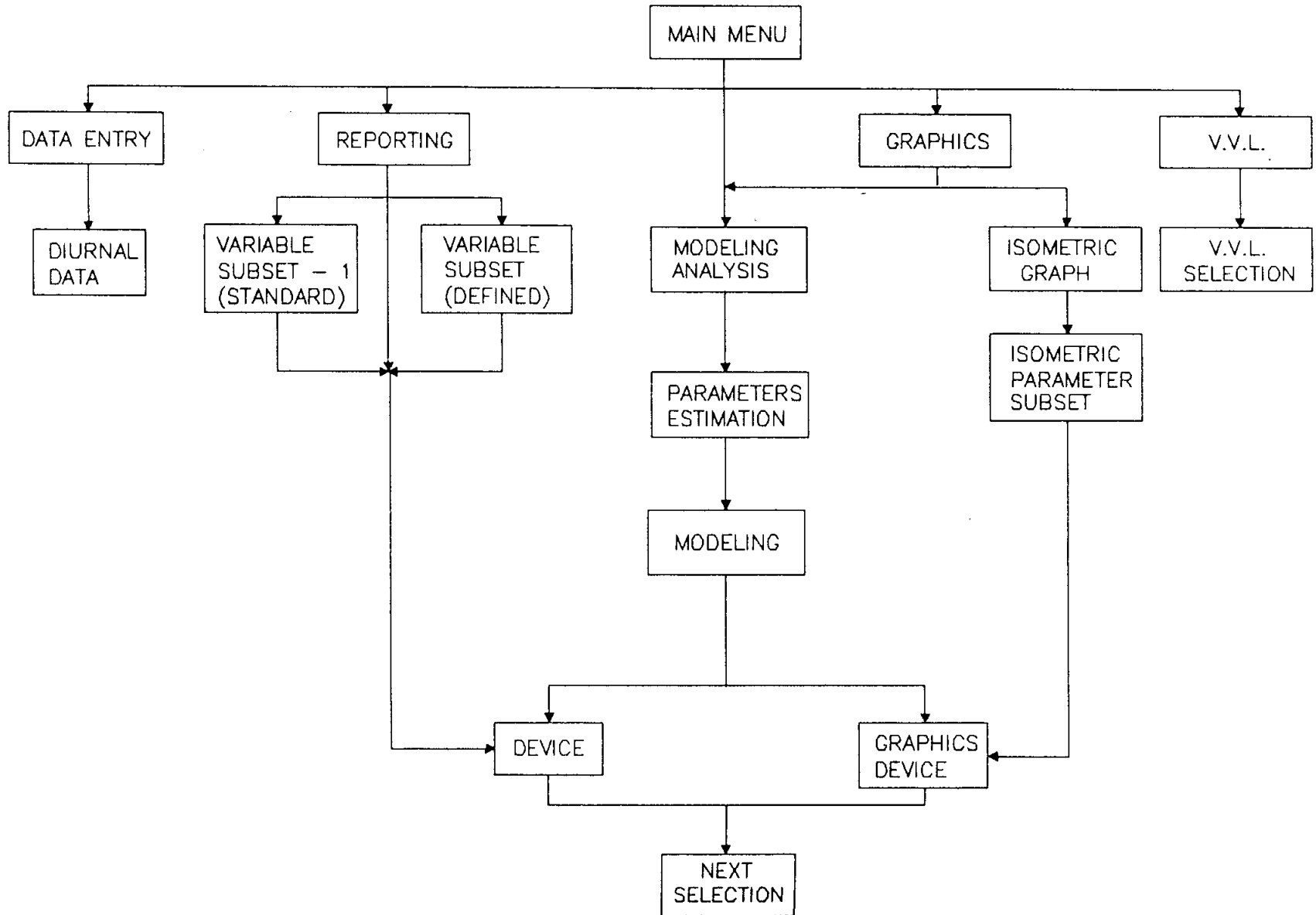
3.2 Data Reporting Module

This module allows access to the report menus from which users select the data subsets and report formats to be generated.

The users can select the data subsets and manipulate data files and data elements through data subset selection screens. This module provides the flexibility for a general report format or customized report. The users can generate as many reports as they like from the same data file or generate a report using any combination of data.

3.3 Modeling Module

This module allows access to the modeling menus from which users select the segment of stream to be modeled.

The concentration of dissolved oxygen in stream water is considered the significant parameter in characterizing stream quality. Water quality standards and regulations are primarily based on the concentration of dissolved oxygen (D.O.). The D.O. balance of stream water depends on factors such as, organic loading, deoxygenation in spatial D.O. distribution is usually observed downstream of the wasteload discharge. Photosynthetic activities of aquatic plant communities produce diurnal fluctuations of dissolved oxygen.

This module provides mathematical formulation of simulating the effect of these factors on the D.O. concentration of river waters, particularly with respect to photosynthetic effect. The module evaluate D.O. concentrations in rivers and simulates the carbonaceous biochemical oxygen demand (CBOD), as well as nitrogenus biochemical oxygen demand (NBOD) at any specified interval along the stream throughout the 24-hour cycle.

SAS/STAT is used for linear and non-linear regression analysis to conduct diurnal D.O. curve analysis and reaction rates.

On the study, CBOD is calculated by a non-linear regression technique. The functional form of

$$BOD = CBOD * (1 - EXP (-Kd * DAY))$$

is applied where

CBOD is the asymptote of the curve,

DAY is the day of incubation in a nitrogen-suppressed long-term BOD test, and

Kd is the deoxygenation rate coefficient,day^{-1}

The linear regression technique is used for computing the total CBOD removal rate coefficient, Kr, and the nitrogenous decay rate kn.

The diurnal D.O. curve is simulated by a Fourier Series mathematical function as follows:

$$D.O. (t) = (A0/2) + A1*COS (3.1416 *t/12) + B1* SIN (3.1416 *t/12)$$

where

D.O. (t) is time variable dissolved oxygen, and

A0, A1 and B1 are Fourier Series coefficients.

The values of coefficients A0, A1 and B1 are estimated by linear regression. The other rate coefficients are calculated by appropriate formulas.

The computed and estimated rate coefficients are utilized in the modeling to simulate the stream conditions observed during the sampling survey.

High resolution regression curve display is optional in this module. Figure 2 shows schematic diagram of the model/database interface.

3.4 Graphics Module

The module allows one to choose high resolution displays of contour, three dimensional plots and bar charts on a specific data type.
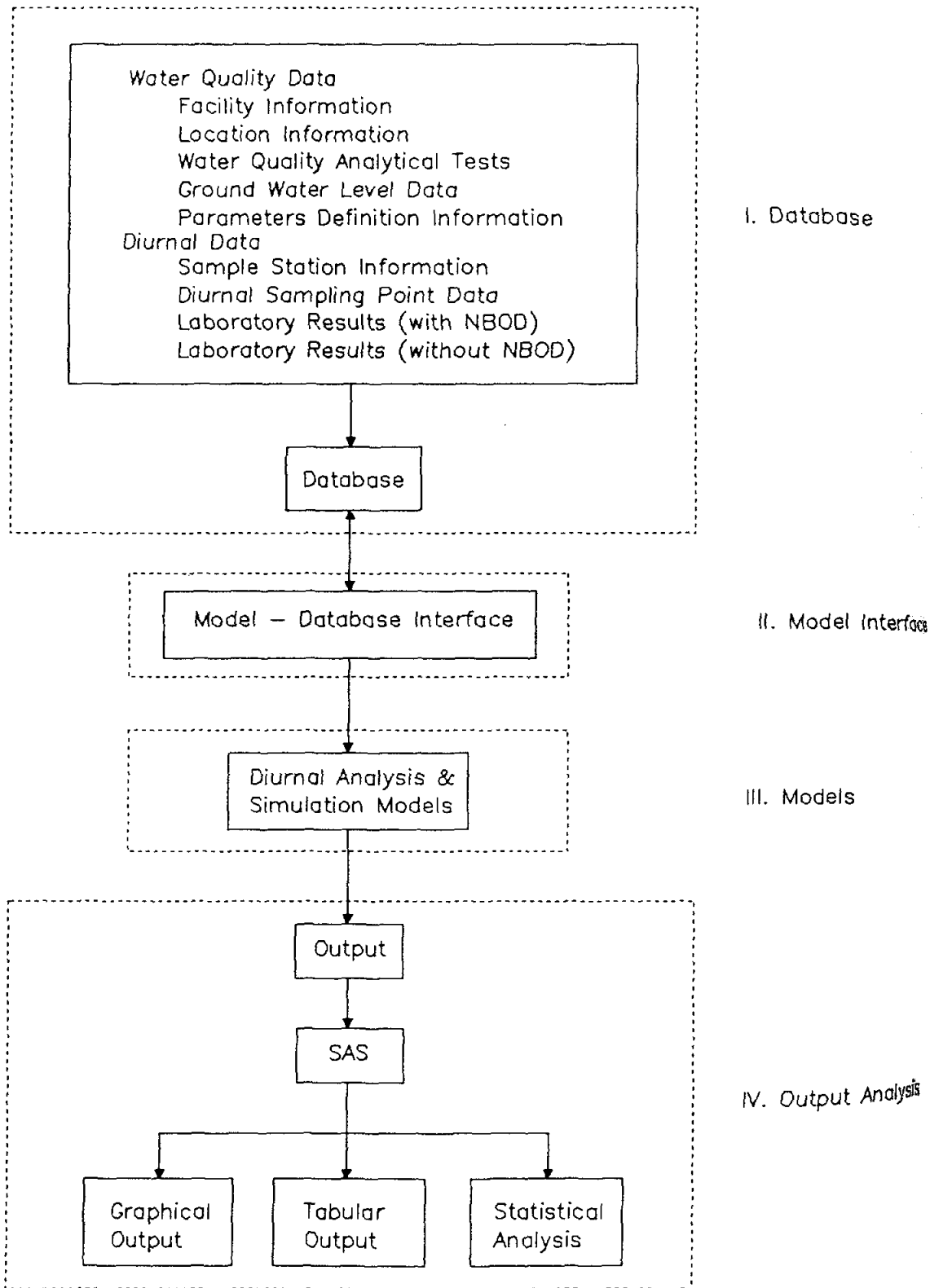
```
                                  Water Quality Data
                                       Facility Information
                                       Location Information
                                       Water Quality Analytical Tests
                                       Ground Water Level Data
                                       Parameters Definition Information          I. Database
                                  Diurnal Data
                                       Sample Station Information
                                       Diurnal Sampling Point Data
                                       Laboratory Results (with NBOD)
                                       Laboratory Results (without NBOD)
```

Database

Model — Database Interface   II. Model Interface

Diurnal Analysis & Simulation Models   III. Models

Output

SAS   IV. Output Analysis

Graphical Output   Tabular Output   Statistical Analysis

FIGURE 2 SCHEMATIC DIAGRAM OF MODEL — DATABASE SYSTEM

SAS/GRAPH, a versatile graphics system for generating a variety of graphics and analysis results, is used as the graphics generating routine for displaying water quality data or diurnal curve analysis in the form of color plots, charts, regression line/curve, contours or 3-D surfaces. Graphics output from this module can be transmitted to one or more of the following devices:

- Graphics displayed on a PC monitor,

- Graphics sent to a device (usually a printer or plotter) attached to a parallel or serial port.

3.5 Valid Value List

This module allows one to browse a list of valid values for specific variables. A Valid Value List (V.V.L.) is a special data type used for looking up coded values for certain variables and/or for validating these coded values against a data file. A V.V.L. data file consists of a coded version of the valid value to be stored in various places in the data structure and a long expanded version of the valid value to be used in reports.

Figure 3 shows the examples of data entry screens. Figure 4 shows the examples of functional selection screens and data subset selection screens. Figure 5 shows the examples of outputs from the system.

4.0 Conclusion

This prototype application system has been developed and demonstrated that:

- It provides a useful and powerful tool for engineers to deal with problems of database management, reporting, analysis, graphics and modeling,

- It provides a flexible/integrated application system which can be customized to meet the different/future needs and requirements.

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Footnotes

[1]PC-SAS, SAS/AF, SAS/FISP,Base SAS, SAS/STAS, SAS/GRAPH are registered trademarks of SAS Institute Inc., Cary, NC. U.S.A.

[2]IBM is a registered trademark of International Business Machines Company.

Figure 3   EXAMPLES OF DATA ENTRY SCREENS

Figure 4 EXAMPLES OF SELECTION SCREEN

Figure 5   EXAMPLES OF SYSTEM OUTPUT

OVERCOMING TECHNOLOGICAL DIFFICULTIES IN CONTINUOUS WATER QUALITY MONITORING

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ABSTRACT

Continuous water quality monitoring programs present many difficulties for water resource professionals. These difficulties may include defining appropriate monitoring goals and objectives, program implementation, sample location and frequency, laboratory analysis, data handling and analysis, reporting, and ultimately, data utilization. Most continuous water quality monitoring programs include the measurements of pH, dissolved oxygen, conductivity and temperature. Other parameters less frequently continuously monitored include salinity, turbidity, florescence, ORP, electrical conductance, ammonia, chlorine and a variety of organic compounds. A literature review of the development of continuous water quality monitoring is presented. This paper also reviews common technical difficulties associated with past and present continuous monitoring programs and with current state-of-the-art instrumentation. Program design options and monitoring considerations are presented which may help water resource managers and technicians overcome common difficulties associated with continuous water quality monitoring.

Improvements in the past few years in solid-state sensor technology appropriate for field use have made collection of continuous water quality data more reliable and economical. However, the voluminous amounts of data collected and the reliability of that data can create additional technical difficulties for the water resource manager.

Monitoring goals and objectives can become lost in the attempt to utilize the voluminous amounts of data. Additionally, water quality regulations are changing to frequency of exceedences, instead of a single standard. Continuous water quality data can more accurately assess the frequency of exceedences than less frequent sampling programs. Does the information generated from a continuous monitoring program provide managers with better information or just more information?

Two case studies are presented which demonstrate areas where continuous monitoring programs can be valuable. The first case study demonstrates how common fixed frequency sampling programs designed to provide water managers with the information needed for reservoir management can be inadequate. The second case study examines how continuously recorded temperature data could have altered a management decision to build a cooling plant on a diversion project to protect the designated use as specified by the NPDES permit. (KEY TERMS: continuous, water quality monitoring, solid-state sensors, reservoir monitoring, effluent discharge.)

INTRODUCTION

The goal of all continuous water quality monitoring programs should be to provide the information necessary for qualified and quantified decision making. A continuous monitoring program must be quantitatively defined and systematically implemented in order to produce the kind of information

desired at the program onset. To assure that the data being collected are adequate for quantitative analysis, the continuous monitoring (sample collection, laboratory analysis and data handling) program must be meticulously implemented and maintained. While continuous monitoring may appear to be an easy way to meet program goals by collecting large amounts of data to satisfy a statistically quantified sample population, many technological difficulties have aggravated the attempts by individuals and agencies to achieve this goal. Although continuous monitoring can produce voluminous amounts of data, the quality of the data collected is often poor. Data analysis, reporting and utilization becomes a management task quite different in scope from the usual situation of an inadequate amount of data. Statistical analysis of continuous data takes on a different role, not as a tool to define a biological, physical and chemical system (distribution, means, variances, standard deviations, etc.) but as a tool for which utilization of statistical analysis is not yet adequately defined.

A good definition for continuous monitoring has yet to be established. However, for this paper we will define continuous monitoring as the automated collection of water quality data at a frequency greater than once per day. The use of solid-state sensor technology allows for nearly instantaneous assessment of water quality. Through the primary use of advanced solid-state sensor technology and microcomputer systems technology, continuous water quality monitoring has improved significantly over the past few years. Some of the technical difficulties in continuous monitoring technology have been overcome with varying degrees of success. However, other difficulties must be overcome through proper program design, data analysis and reporting, and utilization in order to produce the information needed in decision making processes.

LITERATURE REVIEW

Continuous water quality monitoring programs were first implemented in the late 1960's and early 1970's. Continuous systems were developed in Japan, Russia, Finland, England, Italy, France, Germany, Canada, and the United States, among others. Major difficulties were experienced with these systems. Sensor technology for monitoring water quality was being developed and tested in the field. Data handling, transmission, and storage were technical obstacles to overcome.

Many of the technological and practical difficulties associated with continuous water quality monitoring have been overcome in the past few years. It is presently possible to achieve reliable, continuously-recorded water quality data through a continuous recording system network.

Historic Development of Continuous Water Quality Monitoring - A Global Perspective

Sensor technology and monitoring equipment have been utilized around the world for remote water quality monitoring for approximately 20 years. Many articles have been written which describe the application and use of sensors and monitoring equipment and the limitations associated with these systems. The literature reviewed was obtained from an extensive computerized data base search of water resource and chemical technology journals. The literature reviewed included solid-state sensor technology, remote and on-line analyzers, organic analyzers as well as continuous biomonitoring.

Briggs (1978) describes an automated wet chemical method for on-line analysis of total organic carbon (TOC), and chemical oxygen demand (COD) but concluded that the equipment is expensive and difficult to maintain in the field. Briggs also described current limitations in sensor technology and stated that recent developments in ion-selective electrode (ISE) technology may make on-line monitoring practical in the near future. He also described two possibilities for monitoring of organics; GC/MS systems, or ion-selective electrodes capable of detecting organic compounds in water.

Electrochemical sensor technology development has been summarized and described (Davenport 1981; Kalvoda 1984;

Kopancia 1984). At present, the electrochemical organic content (EOC) analyzer is in the experimental phase and many interferences exist (Davenport 1981; Kopancia 1984). Thurnau and Metcalf described use and application of sensor technology. Ion-selective electrodes have shown tremendous potential in the area of continuous water quality analysis for parameters such as alkalinity, calcium, chloride, fluoride, hardness, nitrate, conductivity, temperature and pH. However, problems with ionic strength and interferences with sensor response still need to be worked out (Thurnau 1978; Metcalf 1984). Comparisons of three data-logger and sensor systems to lab instruments which were calibrated in a field test revealed random recording errors for every data-logger and complete sensor failure for some systems. (Metcalf 1988).

Real-time water quality monitoring systems in England have been described by a number of authors. Real-time monitoring systems have been implemented on the River Lee (Wakeford 1978), the River Wear (Wallwork 1978), the Thames Estuary (Cockburn 1981; Ironmonger 1984) and the River Thames (Hinge 1980). Whitehead (1984) described a water quality monitoring station used for input to models used in river water quality forecasting for the Bedford Ouse River Basin in Southeast England.

Kloeppel (1981) and Plate (1981) described continuous water quality monitoring stations in Germany. The Passavant-Werke station "is equipped with automatic cleaning and calibration and can be monitored remotely by means of an integrated computer via MODEM and telephone connection" (Kloeppel 1981). Plate (1981) described an extensive network of 36 real-time water quality monitoring stations in Niedersachsen, (northern West Germany) with a surveillance center in Hildesheim. The system is designed to provide continuous observation of water quality, to provide early recognition and alarms of water quality deterioration or dangerous situations, and to provide documentation of water quality for the purposes of water resource policy and management.

Kohonen (1981) described the utilization of data from automatic water quality monitoring stations in Finland. Eleven stations have been operated by the Finnish National Board of Waters since 1972 (Kohonen 1984).

The City of Osaka, Japan conducted a model project for continuous water quality monitoring using telemetry in 1978 (Nanbo 1981). As a result of the model project, a regulation was enforced in 1979 which limits all factories with discharges more than 400 m^3/day. Stipulations require exact measurement of chemical oxygen demand (COD) using automatic analyzers such as ultraviolet spectrophotometers (UV), total organic carbon (TOC) analyzers and total oxygen demand (TOD) analyzers. Total data loss is less than 4 percent which is much better than other systems described in the literature (Nanbo 1981). Nanbo offers the following comment on maintenance:

"We consider the best way to keep a high running rate is the establishment of a thorough and sufficiently frequent method of maintenance."

Rosa (1987) described a monitoring system on the River Sile which is one the main sources of water supply for Venice, Italy. Two continuous monitoring stations track water quality for 10,700 meters of canal system between the River Sile and the Ca 'Solano treatment plant. Along the canal system are many industrial dischargers including agricultural return flows from 40,000 ha of intensively cultivated land.

Specific National and International Applications of Continuous Water Quality Monitoring

In the United States, probably the most intensive and well established continuous water quality monitoring system is on the Lower Fox and Upper Wisconsin Rivers (Weckwerth 1975). Eleven continuous monitoring stations have been operated by the Wisconsin Department of National Resources since 1971 (Frenske 1988). Since that time many modifications have been made including extensive computerized river forecasting of biochemical oxygen demand (BOD) loading

(Fenske 1988). This network is currently operational and is managed by the Wisconsin Department of Natural Resources (WDNR) in Madison, Wisconsin. The network began operating in 1971 and consists of 11 continuous monitoring stations on the Upper Wisconsin and Lower Fox Rivers (Weckwerth 1975). The major industries on the Wisconsin and Fox Rivers are pulp and paper mills, and hydroelectric plants. Water quality parameters that are monitored include pH, dissolved oxygen, temperature, conductivity and turbidity. Continuous monitoring was necessary to document improvements in water quality which were expected to occur as pollution abatement programs were established.

Major problems with the system included fouling of the sensors, sensor drift, calibration, and electrical interferences. Many of these problems were partially overcome by intensive maintenance and installing automatic cleaning cycles using hypochlorite solutions and air jets. Many modifications have been made since the water quality monitors were first installed, including the use of micro-processor based data-loggers which can provide local processing of data, controlled automatic sensor calibration and self cleaning, and elevated pumping rates. Data are down-loaded from the data-logger to a personal computer and then up-loaded to a main frame for data storage, handling and river modeling. Weekly summaries of data are prepared and provided to department engineers.

A more recently installed continuous water quality monitoring station is presently being operated by Central Arizona Project (CAP) in cooperation with the Bureau of Reclamation in Arizona. This continuous monitoring station has been operational for approximately three years. The CAP station monitors five water quality parameters which include temperature, pH, conductivity, dissolved oxygen and turbidity. These parameters are monitored on a continuous basis with data being transmitted to the CAP Programmable Master Supervisory Control (PMSC) system at regular intervals. Instantaneous readings can be obtained through a voice synthesized recorder by dialing a direct number over standard phone lines.

In general, the CAP water quality monitor has performed very well. However, an intensive maintenance and cleaning schedule is fundamentally important in keeping the monitor and probes clean and operational. During the summer months, maintenance and calibration of the instrumentation is increased from every two weeks to every week (Varner 1988). To help prevent fouling of the sensors and flow cells, the water quality monitor is operated with an automatic self cleaning cycle once a day. Other maintenance includes pump rehabilitation twice a year. Special modifications to some of the electronics in the water quality monitor were necessary due to the high temperatures inside the station.

Sixteen national and international continuous monitoring systems were reviewed in detail, but are beyond the scope of this paper. In general, all continuous monitoring programs investigated suffered from very similar technological difficulties.

Many other continuous monitoring systems and networks have been operational in the United States; however, the available literature is limited. Personal communications were made with dozens of researchers, field technicians, and program managers about their experience with continuous monitoring systems. The federal and state agencies contacted include the Environmental Protection Agency, U.S. army, U.S. Geological Survey, U.S. Army Corps of Engineers, Bureau of Reclamation, and several state Water Quality Control Boards.

The general conclusions reached upon completion of the literature review and personal interviews are as follows:

1) Many water agencies, both national and international, have implemented continuous recording water monitoring programs.

2) Sensor fouling, drift and failure (early years) was tolerated by some of the more aggressive water users

realizing the value of continuous water quality data; others abandoned their programs.

3) Literature describing system failure and program abandonment is limited.

4) Newer technologies and sensor improvement in the mid-1980s have led to the improvement and implementa-tion of many continuous water quality monitoring systems around the world.

5) New sensor technology and improvement in engineering design has not solved all maintenance problems but has made data much more reliable and continuous systems more feasible. Solid-state electronics have greatly improved the performance of monitoring and data logging.

6) Recent changes in regulations by federal and state authorities (especially the Water Quality Act and Safe Drinking Water Act) will require more stringent monitoring of effluent waste streams and potable water supplies in the near future.

7) Portable and mobile organic detection instruments and laboratories have promoted wide spread application of simplified methods for remote screening and preliminary identification of organic contamination in the environment.

8) Many customized organics detection and monitoring systems have been developed for industrial process waste streams. Knowledge of background organic compound concentrations has made detection of elevated levels and unknown compounds possible.

9) A limited number of technologies exists for the continuous monitoring of organics in remote locations. However, the technology that is available has proven to be reliable and requires little maintenance as

compared to on-line or analytical laboratory instrumentation.

10) All continuous surface water quality monitoring stations require individual engineering design and customizing in order to meet specific system objectives and goals.

11) Advances in biological monitoring in recent years has brought this technology out of research and development stage to a commercially available and technologically feasible system. The major limitation in using biomonitors as sensors which relate to human health is that only acutely toxic contaminants can adequately be detected. Chronic levels of contaminants could go undetected or interfere with the interpretation of the results.

EXISTING AND DEVELOPING TECHNOLOGY

Developing Technology

Innovative designs in sensor technology and chemical detection systems have revolutionized monitoring schemes for surface water, ground water, soil, and air, and have saturated the marketplace with new instrumentation. Many of the new detection systems designed in the past few years have yet to be adequately field-tested, which will lead to refinement of engineering design and eliminate poorly designed instrumentation. Some of the re-designed ion-selective sensors such as pH and DO have gained acceptance under the most stringent and controlled in-situ testing, including prolonged applications in corrosive and fouling environments (Hill 1988; Miller 1988; Mullens 1988). Other sensors such as electrochemical organic carbon (EOC) sensors and fiber-optic chemical sensors (FOCS) have not been tested extensively. These new applications could become feasible in the near future (Kopancia 1984; Milanovich 1986; Milanovich etal. 1986; Milanovich 1988).

Increased legislation and public concern for the monitoring of surface and ground

and soil and air for organic pollutants have led to rapid growth of process and on-line organic analyzers, detectors and a variety of analytical instrumentation. These include total organic carbon (TOC) and total organic halogen (TOX) analyzers, electrolytic conductivity detectors (ECD), ion trap detectors (ITD), infrared (IR) detectors, ultraviolet (UV) detectors, parameter specific hydrocarbon sensors (Reidler 1988) and accumulative sampling of trace pesticides and other organics in surface water using a macroreticular cross-linked polystyrene resin such as XAD-4 (Woodrow 1986).

Existing Technology

Most of the state-of-the-art continuous monitoring technology available today in the market place is not "new," rather, current technology has evolved. The literature review brings us up-to-date on the broad applications of continuous monitoring. Our focus under the heading "Current Technology" is on remote or field applications of continuous water quality monitors. State-of-the art continuous recording water quality monitors currently available in the United States are manufactured by Hydrolab Corporation, *Schneider Instrument Company*, Martek Instruments, Inc., and Sierra-Misco, Inc., among others. (Note: the reference to specific manufacturers or use of trade names does not imply endorsement). The basic water quality monitor is most commonly configured to record measurements of pH, dissolved oxygen, conductivity and temperature. These instruments have been used with varying degrees of success and reliability depending on the monitoring program application. Depending on the hardware interface, most monitors can store data on a data logger or remote computer and transmit data over RF, infrared, telephone, hard wire, microwave, satellite, or meteor burst communication links. The most common applications today for continuous water quality monitors is as an in situ remote device interfaced with a data logger to obtain unattended water quality measurements or as a portable field sensor for obtaining multi-parameter measurements of water quality through one instrument. The first application is commonly used for effluent discharge regulatory monitoring or stream water quality monitoring. The latter application is commonly used for reservoir, lake and ocean monitoring.

Common difficulties associated with the use of these continuous monitors are: 1) fouling of the individual sensors, particularly pH and dissolved oxygen, 2) minimal modularity for replacement of individual sensors, 3) insensitivity to low ionic strength and/or cold waters, 4) fixed interval recording limitations, and 5) drift in calibration over long (days to months) periods of time. While not all of the current monitors have the same limitations, some manufacturers are providing water quality monitors with specific sensors for low ionic strength waters or for sensitive DO measurements.

Not all the difficulties previously mentioned have technological solutions. However, monitoring system design and implementation can overcome many of these difficulties. It is the monitoring system design and application of continuous water quality monitors which is the focus of this paper.

Evaluation and Testing

In the last two to three years, the market place has been saturated with new instrumentation for water quality monitoring. Market saturation has made it difficult and costly for program managers and monitoring system designers to economically select a reliable water quality instrument. With the advance of sensor technology, it is unfortunate that not all new technology is reliable. Many federal, state and local agencies have gone to in-house testing for evaluating new technology. Most often the results of the equipment evaluation is not readily available and when the results become available, they are several years outdated.

The U.S. Geological Survey Hydrologic Instrumentation Facility (HIF), the Environmental Protection Agency, the U.S. Army Corps of Engineers, Instrument Testing Association in Washington, D.C. and large municipalities are some of the more common agencies who test and evaluate water quality monitoring equipment on a regular basis.

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PROGRAM DESIGN

Monitoring Considerations

The ability to select appropriate design procedures is as much an art as it is a science (Sanders et al. 1983). Many assumptions underlie the fundamental design of nearly all water quality monitoring programs. It is these assumptions which are not always clearly understood by monitoring system designers and/or not clearly defined for program managers that cause many water quality monitoring programs to fall short of their expected goals. Continuous monitoring can reduce the number of assumptions incurred in designing a statistically sound comprehensive monitoring program. For example, what is the distribution of the parameter of interest, and subsequently what will be the sampling frequency? While these specific concerns are greatly reduced through continuous monitoring, other concerns are greatly elevated. How good are the data? How frequently should the data be recorded? How frequently should the sensors be calibrated? At what level of error in sensor reading do we correct or discard measurements? These questions and more need to be clearly defined, documented and communicated prior to establishing a continuous monitoring network. It has been our observation that these questions have not been adequately addressed in nearly all past and present continuous monitoring programs. Past monitoring programs have been dominated by technological difficulties such as sensor fouling, data storage and handling limitations and reporting difficulties. The final information product for many of these continuous monitoring programs can easily become lost, particularly when the quality of the data is poor. How should continuous monitoring programs be designed? What role should statistical analysis play? What efforts can minimize technical difficulties such as sensor fouling? What can we expect from state-of-the-art continuous monitoring? How can continuous data be utilized by managers in decision making processes? We will attempt to answer some of these questions or provide recommendations by which quality data can be obtained and utilized from a continuous water quality monitoring system.

Considerations for Ensuring the Adequacy of the Data

Continuous monitoring is not a 'cure all' for obtaining water quality data. Continuous monitoring does however provide a clearer understanding of the natural system we are attempting to describe. The following considerations apply to the use of solid-state water quality monitors as information gathering tools. The incorporation of these recommendations into the network design process will help to ensure the adequacy of the data being collected.

1) Carefully and precisely define the goals of the continuous water quality monitoring program.

2) Select water quality parameters which are indicative of the system you are describing.

3) Select the sensor technology which is capable of measuring the range and reactivity of the system. For example, low ionic strength waters, low range DO waters (<1.0 mg/L), and flashy or slowly changing systems.

4) Consider the modularity of the water quality monitor. Can individual sensors be replaced?

5) Evaluate the calibration technique for each sensor. Do the sensors have temperature correction? Can the sensors be calibrated in the field?

6) Estimate the time required for maintenance and calibration. Can the sensors be easily cleaned? How often will the sensors need cleaning and calibration?

7) Consider the functionality of the data collection device the water quality monitor is to interface with. Can the data collection device be programmed? Does the data collection device have the capability of increasing or decreasing the recording interval based on concurrent changes in the system? What communication

modules can the data collection device be configured to communicate with? Can the data collection device track maximum or minimum values? Can daily or hourly averages and means be computed in the field? Can the data collection device communicate with other outside peripherals such as automated samplers, printers, alarms, modems and backup storage devices? What is the data storage capacity of the data collection device?; does it satisfy the monitoring program objectives?

8) Carefully select the monitoring location. Locate monitoring stations so that the data collected are representative in space.

9) Select a recording frequency that is representative in time.

10) Consider and define statistical procedures which adequately utilize the data being collected (eg. time series analysis, moving averages, number of exceedences per time period etc.)

11) Consider installing two water quality monitors side-by-side. Statistical comparison of 'duplicate' sensor readings can define the quality of the data being collected and assist in evaluating sensor performance.

12) Consider the site specific installation locations. How fast or slow is the water moving? What is the potential for algal growth? What is the potential for vandalism or natural destruction?

13) Consider the maintenance personnel. Do they understand basic electronics? Do they understand water quality systems? Will they recognize warning signs of sensor or other malfunction? Do they understand the project goals? Are they trainable and available? Will they work off hours?

14) Consider the reporting format. What kind of information product do you want? Is the data collection format compatible with standard spreadsheets and data bases? Are tables and figures desired? How much data manipulation will be required to get the information you need for decision making?

These recommendations should be incorporated into the monitoring system design process. The economic realization for the project manager should be fully understood before the project begins. An attempt to implement a continuous monitoring program without carefully considering the above mentioned items can result in a costly and unproductive program which will in -many cases be abandoned. When these considerations and recommendations have been incorporated into the design process, continuous water quality monitoring can be an economically feasible, and informative tool for accessing water quality systems.

CASE STUDIES

Two case studies are presented where continuous monitoring provides a manager with different information than a traditional fixed frequency or event driven monitoring program. Traditional monitoring programs typically use frequencies of days, weeks, months or even years between sample collection. This frequency can satisfy the statistical requirements of the program by collecting an adequate number of samples. However, the samples are generally collected at the same time of day which does give important information on the monthly or seasonal fluctuations, but does not yield information on diurnal fluctuations. Two case studies are provided which demonstrate how continuous monitoring can provide valuable information which is not obtained with traditional monitoring programs.

The first case study is Cherry Creek Reservoir, in Denver, Colorado which was evaluated as part of a project to examine in-lake treatment options for controlling

eutrophication. Cherry Creek Reservoir is a terminal storage reservoir, which is very shallow (average depth of 17 feet), receives significant non-point phosphorus loadings, experiences nuisance algal blooms and has tremendous recreation pressure. The reservoir has been managed by attempting to limit phosphorus input to the reservoir. A limiting nutrient study completed in the summer of 1988 indicated that the reservoir was not phosphorus-limited during much of the summer. The reservoir may have changed from a phosphorus-limited condition of several years past to a light and nitrogen-limited condition over the past several years.

During light-limited periods, fine sediments, which are easily suspended from the reservoir bottom, contribute large amounts of phosphorus to the nutrient pool in the reservoir. Total phosphorus concentrations were monitored several times in one day at the deepest section of the reservoir. The total phosphorus concentrations varied from 77 ug/L in the morning to 224 ug/L in the afternoon. These data indicate that during times of the season when the reservoir is mixing to the total depth due to wind and/or motor boats, total phosphorus concentrations are highly variable throughout the day. Instantaneous data collected monthly or weekly to indicate trends through time are not useful indicators of phosphorus dynamics in the reservoir given the fact that total phosphorus concentrations vary significantly during the course of one day. Also, the variability of total phosphorus concentrations in a day when no significant inflows were contributing phosphorus to the reservoir indicates that there is an abundant supply of phosphorus in the sediments that becomes resuspended. Additionally, phosphorus may be resolubilized if dissolved oxygen concentrations approach 0.00 mg/L and anoxic conditions develop. If the diurnal fluctuations of total phosphorus were evaluated earlier, management of the reservoir would needed to have considered accumulation and resuspension of phosphorus, and possible intake control options such as dredging.

The second case study is a water diversion project which has had temperature restrictions imposed on the diverted water as part of an NPDES permit to protect designated uses of the receiving water. Both the diverted river water and the receiving stream have been monitored for many years. The temperatures of each river at several stations were measured at various times during the day during each sampling date. Diurnal fluctuations were impossible to evaluate until continuous monitoring was used. The receiving river is a much smaller river than the river from which water will be diverted, therefore it exhibits a wider diurnal fluctuation in stream temperatures. The water temperatures in this smaller river also exhibited a much higher flucuation between stations due to shading and tributaries. Continuous data which have been recently collected are essential in demonstrating that the larger river exhibits less diurnal flucuations than the smaller river and is not significantly warmer with respect to achieving beneficial uses in the receiving stream. Therefore, continuous monitoring to monitor the system and manage the diversion to insure that no adverse impacts to fish will occur.

SUMMARY AND CONCLUSIONS

The purpose of water quality monitoring programs is a well defined information product which describes the behavior of a hydrologic system. Carefully designed and implemented, a continuous water quality monitoring program can produce the type of information product needed for critical decision making. The value of the results of continuous water quality monitoring depend on the energy, time and money put into the program. Continuous monitoring does not solve the data collection and analysis problem of a "total" monitoring program. Continuous monitoring does, however, eliminate some of the uncertainties of a statistically described system. Not all monitoring programs need to implement continuous monitoring. However, many monitoring programs could benefit greatly from continuous monitoring. The direct benefit obtained from continuous monitoring is dependent on the underlying assumption that the data collected are of good quality and can be utilized as an information product for decision making.

In most societies, the economics of a monitoring program is the limiting factor in system design and operation. The costs associated with continuous monitoring should be viewed in terms of the overall water system management costs. Many times costly management decisions are made based on an inadequate description or 'picture' of the physical, chemical and biological system.

In conclusion, continuous monitoring has a rightful place in many monitoring programs. Improvements in the past few years in sensor technology combined with properly defined goals, objectives and system design, will make continuous monitoring an important component in comprehensive assessments of the hydrologic systems. With proper maintenance and operation, continuous monitoring will enable water resource professionals to make more appropriate management decisions.

ACKNOWLEDGEMENTS

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Managing Water Quality
Data Records on Computers

ILLINOIS WATER INVENTORY PROGRAM

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ABSTRACT

This paper describes the organization and capabilities of the Illinois Water Inventory Program (IWIP) databases; Public-Industrial-Commercial Survey (PICS), Surface, County, Discharge, and Lab number; and their interaction with Illinois State Water Survey (ISWS) ground-water quality database (GWQDB) and geographic information system (GIS). The IWIP was initiated in 1978 as an effort to bring together our state's diverse collection of water information. The PICS database, developed within this program, is a site-specific database that contains information about high-capacity wells or intake points. It utilizes a standard query language relational database management system to store and retrieve information. The key file in this database, "point source", contains water withdrawal point location information and identification numbers or names used at the ISWS and at other state and federal agencies.

Information such as quantity of water withdrawn, water quality lab analysis numbers, analysis date, unique identification numbers for use in GIS applications, water sources, owner/operators, well construction details, and populations served is related back to the "point source" file. This feature allows flexible querying of the database. Data are entered through interactive query forms or by batch processing. Output from the system queries can be sent to the screen, to computer files, or to a printer. Output reports range from unique questionnaires for each major water withdrawal to input data files for processing by a GIS mapping system.

INTRODUCTION

Increasing demand for domestic, agricultural, and industrial water, along with water pollution and droughts, makes it necessary to document current water quality and uses to facilitate effective planning and proper management of Illinois water resources. In 1978, the Illinois State Water Survey (ISWS) worked with the U.S. Geological Survey to expand previous water use data collection activities to include all areas of Illinois and all water sources. The Illinois Water Inventory Program (IWIP) documents the state's water use. The data are used to help manage ground-water resources in the northeastern part of the state, where a major ground-water resource system is currently being "mined"--that is water is being withdrawn faster than it can be recharged. The water use information benefits other state agencies and compliments resource-related research and studies. The ability to aggregate various regional water use patterns rapidly makes it possible to plan for the most effective use of Illinois water resources for economic and social well-being.

The Public-Industrial-Commercial-Survey (PICS) is a site-specific database that contains information on more than 10,000 active and inactive high-capacity withdrawal point sources for more than 4600 facilities throughout Illinois. The key file of the PICS database contains withdrawal point location information and other identification and cross-reference numbers or names used at the ISWS and at other state and federal agencies. The database is designed to show changes in quantities

of water used, to indicate trends in use, and to provide the basic data required for establishing water budgets and developing water use plans. The database includes all public water supply wells and intakes and high-capacity (more than 70 gallons per minute) wells and intakes for industries, commercial establishments, and fish and wildlife management areas. The PICS also contains a mailing address file, detailed well and intake information, annual pumpage, and water-level information. Other IWIP databases contain data elements such as stream code, drainage area, impoundment information, county population projections and area, National Pollution Discharge Elimination System (NPDES) numbers and discharge, lab numbers and dates which all can be related back to the PICS.

The ISWS began its effort to survey the quality of Illinois water resources in 1895. A preliminary report, Chemical Survey of the Water Supplies of Illinois (Palmer, 1897), was the first ISWS publication (ISWS Bulletin 1). Since the early 1940s, the ISWS has increased its evaluation of the withdrawal of Illinois water resources. Most previous ISWS reports on water use emphasized those regions of Illinois where water resources were extensively developed; such as Chicago, Peoria-Pekin, E. St. Louis, and Rockford areas; or they surveyed withdrawal by major use categories. The IWIP databases build on these and extend earlier efforts to all areas of Illinois.

The ISWS Ground-Water Section is the State central repository for an estimated 500,000 ground-water analyses, water well records, and engineering reports, as well as some surface-water-related information. The oldest known well included in the PICS database was dug in 1754.

Municipal water supply reports in Illinois have been published since 1907 (Bartow, 1907), culminating with the present ISWS Bulletin 60 Series (Woller, 1989). This series of publications documents the history of ground-water development within each county of Illinois. Similar information for surface water is presented in ISWS Contract Report 442 (Singh, 1988). Industrial, commercial, irrigation, and conservation area pumpage

reports were initiated in the mid-1940s. A 1988 publication on water withdrawals in Illinois is now in progress.

DATABASE ORGANIZATION

In 1978, the IWIP began as an effort to organize the diverse collection of Illinois water information into a computerized format and provide aggregated data for the U.S. Geological Survey's National Water Use Data System. Water withdrawal information was obtained yearly from a unique questionnaire sent to each water user included in the database. In the first year of the program, the collected data consisted of total pumpage for each public water supply or large industrial water user (more than 70 gallons per minute). Additional information, such as individual withdrawal locations and aquifers utilized, was included to make the IWIP databases a more useful and accurate source for water information.

The original IWIP "Water Use" database was compiled from a list of large employers supplied by the Illinois Department of Labor, a list of public water supplies provided by the Illinois Environmental Protection Agency, and a search of the ISWS water resource records. This information was maintained on the University of Illinois at Urbana-Champaign CYBER-175 mainframe computer system and consisted of three files linked by a facility identification number.

The three files were generally referred to as "mail," "use," and "support" files and by 1980 they were supplemented by the development of procedure files and FORTRAN programs. These programs were used to produce output ranging from unique questionnaires for each facility, to computer-generated photo-typeset summary data tables ready for publication.

The IWIP database files were very useful but difficult to update. To facilitate rapid data retrieval, all files carried the name of the facility, a facility identification number, and some location information. Updates and changes were made with a line editor, and in many cases all files had to be edited.

In 1984, this database was moved to an Altos 986 multi-user microcomputer. The data structures remained much the same, but a new data entry procedure was developed. An interactive entry program created an input file that was used for batch updating of the database files. The PICS database was established with the acquisition of a standard query language (SQL) relational database management system (INFORMIX-SQL) for the Altos microcomputer. The database size increased to include new data files, data elements, and extensive indexing for data retrieval.

The PICS used earlier "mail" and "use" files with minor additions. The original "support" file became PICS "point source" and "withdrawal" files, with the addition of more locational data elements and cross-references to other state, federal, and GIS coverage identification numbers. A new file, "water level," was added to round out the PICS. The annual survey verifies most of the PICS information and adds annual information. Related files dealing with information not directly collected by the survey (Surface, County, Discharge, and Lab number) comprise the rest of IWIP databases (figure 1). These files include data elements such as stream code, drainage area, impoundment information, county population projection and area, NPDES numbers and discharge, lab numbers and dates linked back to the PICS.

The GWQDB is a compilation of the reports of chemical analyses performed by the Illinois Environmental Protection Agency (IEPA) and ISWS laboratories from well water samples collected in Illinois since 1895. There are approximately 44,000 analyses in the database; about half are from Public Water Supply wells and the rest from private wells. The bulk of the data is from the period 1970 to present. Before 1987, most analyses were for inorganic compounds and physical parameters. With 204 files, each containing data for either public or private wells for one of the 102 counties in the state, maintenance of the GWQDB created the need for another Altos 986 computer. An interactive querying program has been developed to allow for frequent small-scale use and response to requests.

ARC/INFO is the GIS used to manipulate and display geographic data as maps or coverages. Point, line, and polygon coverages of areas of interest in Illinois are created and maintained on a PRIME 9955-II computer. The coverages used most often with the IWIP data include public water withdrawal points, aquifer potential yield, lakes and streams, county and township, and transportation and utility corridors.

The IWIP database files are related by ISWS facility/withdrawal point identification numbers (figure 2), to the GWQDB files via lab numbers, and to the GIS database coverages via point and township polygon identification numbers and locational coordinate data (figure 3). Information such as quantity of water withdrawn, unique GIS identification numbers, lab numbers, water sources, owner/operators, well construction details, and population served can all be output according to individual research requests.

DATA SYSTEM CAPABILITIES

Input to the system is accomplished through interactive entry forms or through batch processing. Database query outputs can be sent either to the screen, to a printer, or to a computer file. Custom reports range from unique questionnaires for each major water withdrawal to complete files for use with the GIS system.

The PICS database is regularly updated. Mailing and withdraw point files are combined to produce annual withdrawal questionnaires. Each computer-generated form is unique to the facility and includes withdrawal source information categorized by the general type of water use. Five types of questionnaires are produced: 1) public water supply, 2) electric power generation, 3) institutional, 4) conservation lands, and 5) industrial/ commercial. The forms are processed upon return and compared with data from past years. Any substantial change is verified with the facility. The database is updated using interactive INFORMIX database screen forms, in which the layout mimics the structure of the questionnaire. During

County Info (IWIP)	Water Levels (PICS)	Industrial Use (PICS)
Withdrawal Info (PICS)	Point Source Info (PICS)	Mail Info (PICS)	Discharge (IWIP)
Surface Info (IWIP)	Lab Number (IWIP)	Public Use (PICS)

County #   Facility/Point id   Facility id
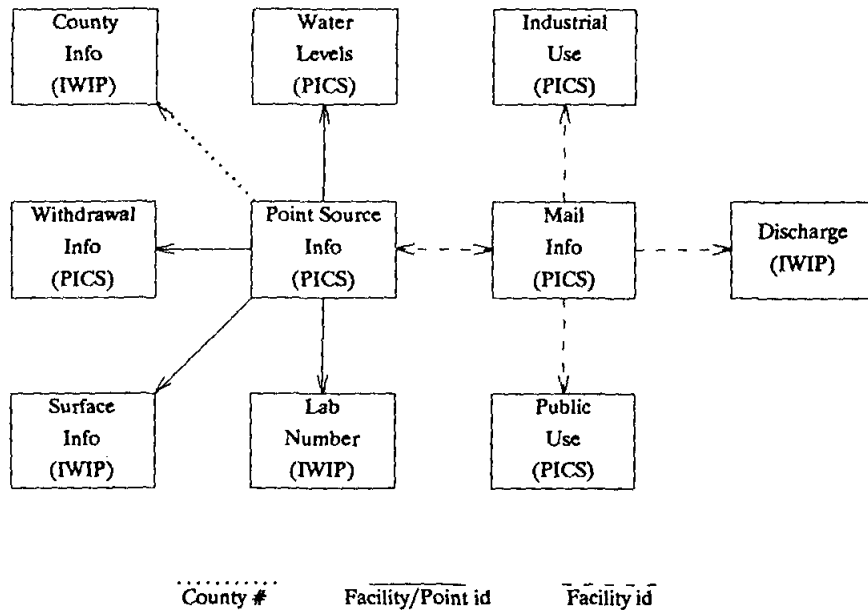
Figure 1. IWIP file structure with ID links

Mail Facility ID Name Contact Title Address Phone Nos. ... ... -etc-	**Use** Facility ID Self-supply Q Purchased Q Population ... ... -etc-	**Point Source** Facility ID Point ID SIC code Water Source Location Data Other IDs Construction Data County No. ... ... -etc-	**Withdrawal** Facility ID Point ID Max Daily Q Annual Q -etc- **County** County No. Name District SMSA Sq Miles Populations ... ... -etc-	**Water Levels** Facility ID Point ID Non-pumping level Pumping Level Pump Rate ... ... -etc-	**Lab Number** Facility ID Point ID Analyses Date Lab Number Analyses Count ... ... -etc-	**Surface** Facility ID Point ID Stream Code Impoundment Info Drainage Area ... ... -etc-	**Discharge** Facility ID NPDES No. Stream Code Location Data Discharge Q ... ... -etc-

Figure 2. Join relationships in IWIP databases
(potential join columns shaded)

GIS Facility ID Polygon Area Polygon # GIS Point ID -etc-	**Point Source** Facility ID Point ID Polygon # Unique ID Location Data SIC Code Other IDs Construction Data County # -etc-	**Lab Number** Facility ID Point ID Analyses Date Lab Number Analyses Count	**GWQDB** Municipal # Well # Analyses Date Lab Number Analyses -etc-
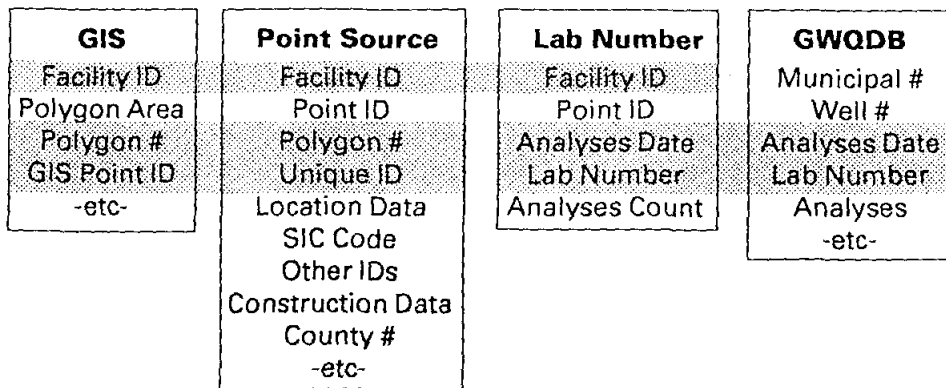
Figure 3. Join relationships with IWIP, GWQDB, and GIS
(potential join columns shaded)

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this procedure, annual water with drawal information and changes are entered into the database.

After completing the annual data collection, a water withdrawal summary is produced. These summaries are computer-processed to produce camera-ready, typeset tables for standardized publications.

The database allows batch unloading or loading of ASCII files for exchange with other databases. Interactive "forms" also can be used for small queries of the database. Each form consists of one or more screens of information obtained from up to 14 database files. Specialized forms are used to respond to many information requests in which the data elements can be explained as part of a 22-line, 80-character screen (figure 4). For larger information requests, the database management system has a "report-writer" generator that can produce custom-formatted reports. The report program allows for greater flexibility in the type and complexity of the database query and the detail of output. The only limits for these customized reports are temporary file storage, output device capability, and time.

The GWQDB is updated from computer tapes of chemical analyses from the IEPA and ISWS laboratories. The GWQDB is maintained as 204 files each containing data for either public or private wells for one of the 102 counties in the state. An interactive querying program was developed to allow for frequent small-scale use and response to requests. Called "query," the program extracts information from the GWQDB. Users are asked to specify public water supply data, data from private wells, or treated water samples. The data contains information about the wells (county, location, municipality number, well number, depth, old aquifer code, new aquifer code) and the sample (sample date, laboratory number, sample type), followed by the concentration levels, (usually in mg/L), for up to 61 parameters. Subsets of the data may be chosen based on location, municipality number, well number, depth, new aquifer code, year of sample, and/or parameters. One to sixty-one parameters may be requested. The same subsets and parameters are

examined for each county specified in each execution of query.

The geographic information system managed on the Illinois Department of Energy and Natural Resources (IDENR) PRIME computer is used for mapping and plotting information (figure 5). To facilitate the use of the GIS capabilities, the PICS database carries township polygon identification numbers, withdraw point map identification numbers, and Illinois Lambert Conformal Conic Projection coordinates. These three elements provide quick access for GIS application.

HARDWARE

The IWIP databases and GWQDB reside on the Ground-Water Sections Altos Network, three Altos 986 computers running the Altos XENIX 3.0 runtime and development operating system and WorkNet, with PC-Path and MS-FORTRAN. An IBM PC/AT and an AT&T 630 share a desktop typesetting system, EROFF, on Altos partitions and a HP LaserJet II via PC-Path. The GIS is ARC/INFO and resides on a PRIME 9955-II computer running Primos 21.0.5 using the IBM PC/AT as a terminal via Sytek LocalNet, a Calcomp 1051 pen plotter and a Calcomp 9000 digitizer board.

Most data reduction and processing for the IWIP are accomplished through the use of various software packages available on the Altos microcomputer. This system includes an editor (vi) on the Altos, which allows less data manipulation on the IDENR PRIME, and includes a diverse set of XENIX utilities available for data handling on the Altos. Together, these capabilities made the Altos 986 microcomputer the most effective system for IWIP development at the time.

CONCLUSIONS AND FUTURE DIRECTIONS

Lessons Learned

A number of lessons are apparent, being learned with the development of the IWIP databases. One of the most obvious is the need for a unique identifier for use with each

```
--------------------------------------------------------------------
SWS Id#     [00190550]   Well # [1          ]   File # [33]   SIC code [4941]
--------------------------------------------------------------------
Name  PAYSON                        Address   307 N FULTON
City  PAYSON        IL              Zip code  62360
--------------------------------------------------------------------
Status: [1] Location  [00103S07W0888] PM [4]   Lat [3949070] Long [9114300]
Hydro code  [07110004]         Depth  [330        ]    Aquifer code  [3040]
Feet from corner  [1000N 0100E]                        LSD  [763         ]

q86      12893000.00           q87      14842100.00
q88      10822750.00           q89
```

Figure 4. Simple screen form data query output

+ Radium—Alpha
▽ Arsenic
· Fluoride
□ Barium
△ Nitrate

Public Water Supplies
with Wells Failing
Drinking Water Standards
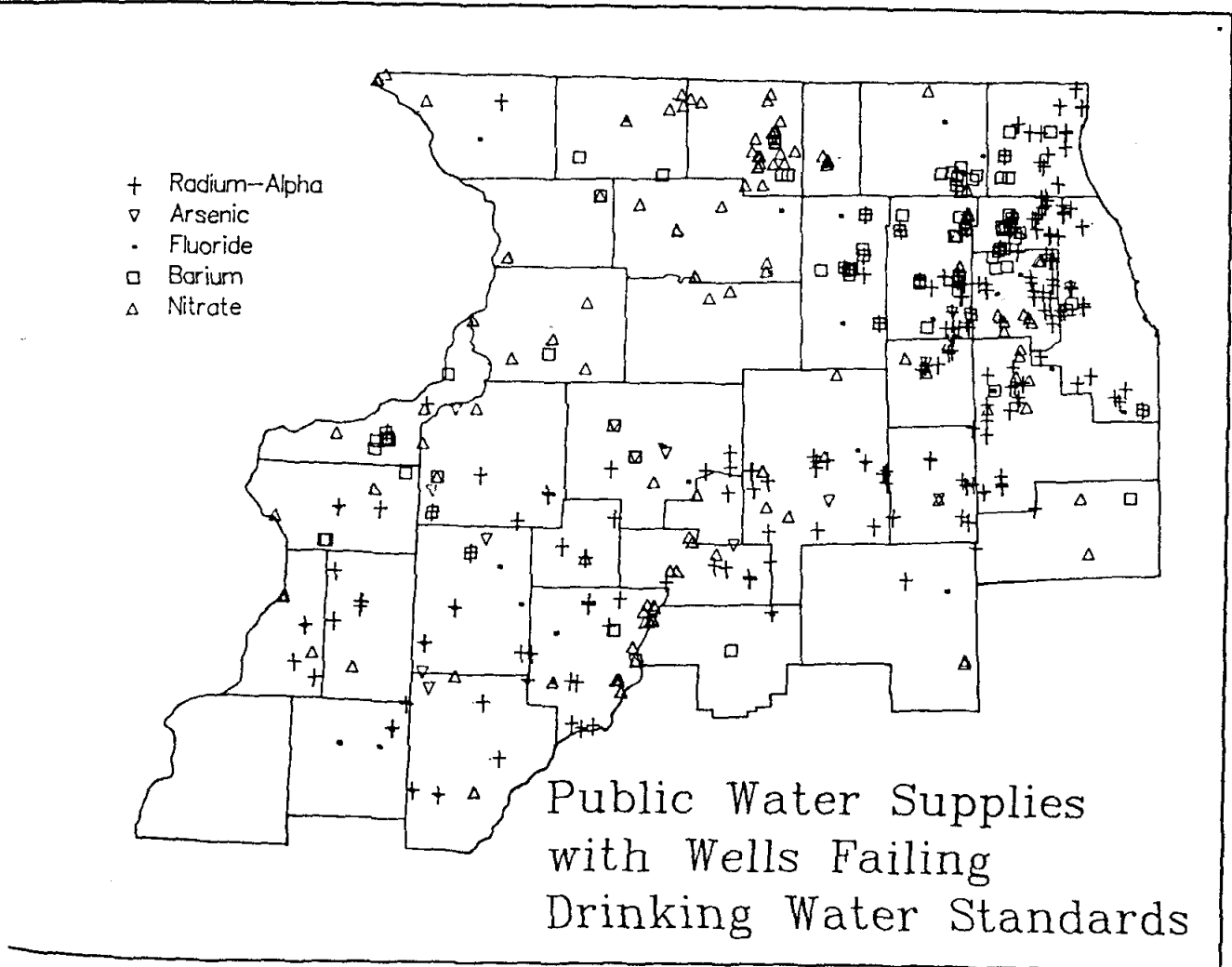
Figure 5. Map output of IWIP, GWQDB, and GIS data

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data record. When possible, cross-referenced names, other identification numbers, and historical information should be included in the database so that other data can be utilized in combination with this information. The simplest way is to let the computer generate a unique ID code, either random or sequential, and NEVER reuse this ID.

GIS system-compatible coordinates should be used for locational reference. Earlier IWIP databases used the U.S. Public Lands Rectangular Survey as a unique locator. Due to some duplication of townships, ranges, and sections within the same principal meridian, Lambert coordinates have been added to the PICS database to overcome possible locational confusion.

Avoid using special extensions in computer program languages in order to make applications transferable. In many cases, the special extensions are not available on different computers or under different operating systems. For example, the early use of CYBER FORTRAN-5 language extensions which are not available in MS-FORTRAN on the Altos minicomputer.

Frequently, databases are designed and created while information is being collected. Major problems with databases often occur during this initial creation process. Extra effort must be taken in designing a database to meet management objectives and goals. The extra time used in planning should result in better data collection.

Care should be taken in terms of data decentralization especially since the personal computer (PC) revolution. It is possible to keep one's own specialized dataset, but the same quality control-quality assurance procedures should be maintained on each dataset.

Verification of data prior to, during, and after entry should be a major consideration in developing a database. In water resource planning, the quality of the data should be more important than the quantity.

Future goals

Currently, the IWIP is planned to become an integral part of an ISWS ground-water relational database system. The withdrawal source data will be expanded to include all reported wells and linked to raw water-quality analyses, a water-level observation network database, and an aquifer properties database (figure 6). As the rest of the water resource records become computerized, a PC networking system is being explored as a means to centralize the ISWS ground-water data into a single database with access to GIS capabilities.

The PICS and Bulletin 60 effort will continue to collect and store data for the IWIP. Through this data collection effort, information concerning Illinois water resources will continue to be documented and utilized.

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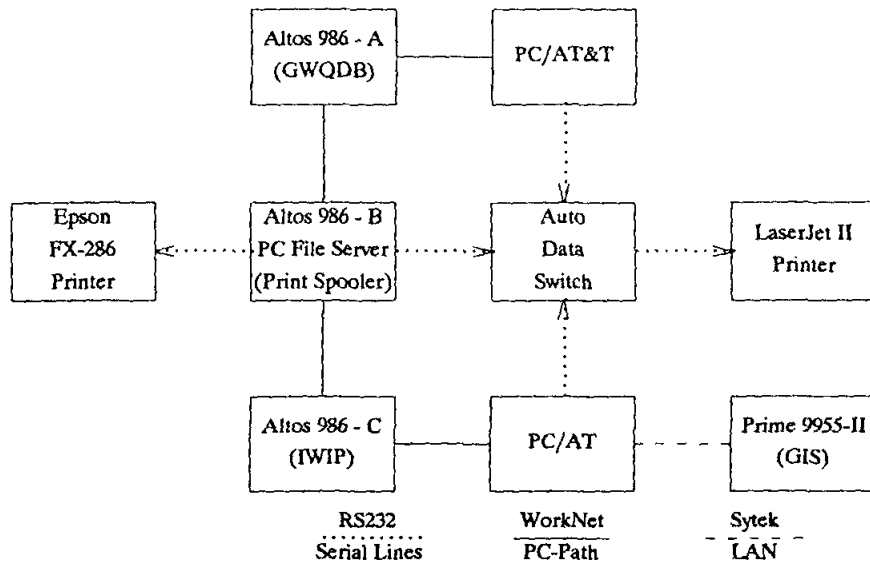
Figure 6. IWIP network structure
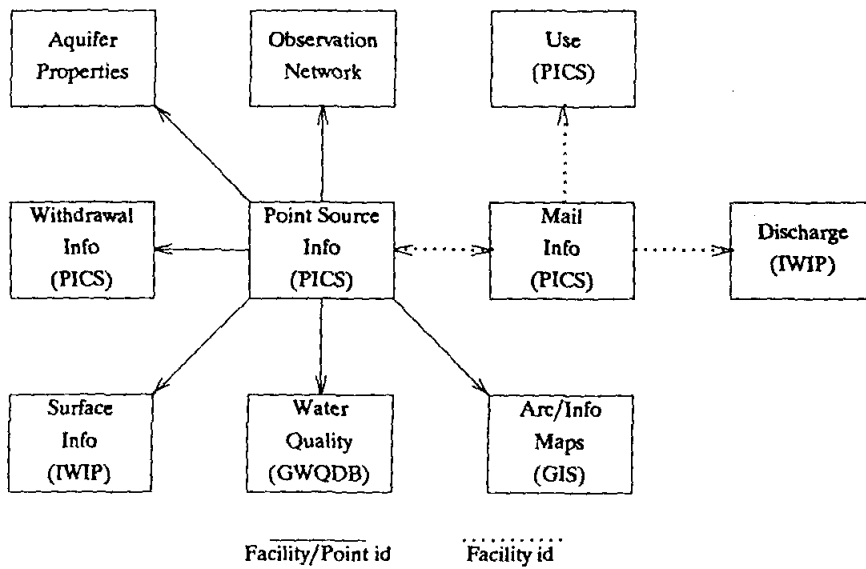
Figure 7. Future database file structure

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NAQUADAT, A REDESIGNED DATABASE

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ABSTRACT

The National Water Quality Database (NAQUADAT) was designed in the late sixties to store information generated by the Water Quality Branch (WQB) monitoring programs. As time progressed, so did water quality information requirements. Water quality monitoring programs have been redesigned to address current issues such as acid rain, pesticides, and dioxins. NAQUADAT, except for a conversion from a sequential tape-driven system to a hierarchical SYSTEM 2000 database-management system, remained relatively unchanged until the present. It has now been completely redesigned. The new NAQUADAT uses the relational database-management system ORACLE, providing easy access for users. It is far more flexible than the old system and can store all types of aquatic environmental information including chemical, biological, and sediment data. Quality-assurance data can also be stored on the database. Access and retrieval of information is via the Structured Query Language (SQL) which can provide standard user views or custom-designed reports.

INTRODUCTION

The NAQUADAT data base was initially designed and implemented in the late sixties (Demayo and Hunt, 1975; Demayo, Lamb and Whitlow, 1986). It was set up as a storage and retrieval system to manage the data from the Water Quality Branch (WQB) monitoring program.

The monitoring program, for the most part, consisted of collecting samples of water from rivers at highway crossings. The samples were shipped to the laboratory and analysed for physical, major ion, nutrient, and a few metal parameters. Data were entered onto laboratory cards and then keypunched onto computer cards. The software, consisting of COBOL and FORTRAN programs, also ran from punched cards. The information was stored sequentially on magnetic tape ordered by Station_number, Date, and Time. Two of the more important features of the database are the station number and the parameter code.

The station number consists of a twelve-character field that contains information on the sample medium, province, basin designation, as well as a sequential number for each station in the same subbasin. The parameter code consists of a five-character field, the first two characters being the atomic number of the element.The remaining three characters indicated the analytical method used.

In 1980, as technology advanced and disk storage (allowing faster direct access to the data) became more available, the NAQUADAT files were converted to use the hierarchical database-management system SYSTEM 2000. The database was maintained on a Control Data Corporation CYBER computer and users were permitted some interactive capability. However this was a straight conversion from a sequential file to a

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hierarchical storage system. No changes were made to the file system concerning record types, field sizes, or data types. TABLE 1 shows the schema of this database as it exists today.

Over this same period, water quality monitoring has evolved considerably. Although networks of fixed sites still exist, the sites are chosen carefully for specific purposes and not just for convenience of access. The suite of parameters measured has grown and includes many organic contaminants. Where appropriate, sediment and biological samples are also collected.

To complement the fixed-station networks, intensive surveys to investigate cause/effect relationships or spatial variabilities are often carried out. Effects monitoring and biomonitoring are becoming more widely used as these programs develop. Toxicological screening tools are also being developed.

Samples upon which the measurements are made no longer consist of one or two bottles of water. We have large volume extractors, resin columns, net hauls (a single net haul can produce several samples), dredges, cores, and composites, among others. Information provided by measurements made on these samples are important to water resource managers and must be managed accordingly. The existing NAQUADAT cannot accommodate this information. It was not designed for this purpose.

BACKGROUND

Database technology has progressed and relational database- management systems (RDBMS) are now the accepted industry standard. Unlike hierarchical systems, relational database systems consist of many related two-dimensional tables. Data can be accessed in many different ways.

In 1988, the computer service centre that Water Quality Branch uses for the NAQUADAT database notified Environment Canada that they were downsizing their operations. They would no longer be supporting the SYSTEM 2000 database-

management system. The Water Quality Branch commenced planning the conversion of NAQUADAT to take advantage of relational database technology.

Historically, computing costs were expensive compared to labour costs and a database had to be as efficient as possible. On occasion, efficiency was at the expense of functionality. Nowadays computing costs are low relative to labour costs. Data storage costs are continuing to fall. Central processing units (CPUs) are becoming more powerful. Desk top workstations capable of operating at 175 MIPS (million instructions per second) exist.

Users of the NAQUADAT system had complained that the SYSTEM 2000 database was difficult to use and anything but user friendly. We decided that the new NAQUADAT would be as flexible, functional, and as user-friendly as possible for the end user, even if this meant losing some efficiency. The new database, although designed primarily for the use of the Water Quality Branch Headquarters, could easily be adopted by the Regional Offices. The system must be flexible enough to permit any office to easily add an extra field or table for a specific purpose. For example, the WQB Pacific Region store information on lay sample collectors for each monitoring site where lay collectors are used. WQB Headquarters will maintain a station cross-reference table. NAQUADAT frequently exchanges data with other databases and this additional information must be stored.

The RDBMS ORACLE was chosen as the database-management system to be used for NAQUADAT. ORACLE was already being used for some Environment Canada databases including a regional water quality database and had been identified as a departmental standard where appropriate. The planned implementation date is January 1990.

DATABASE DESIGN

At this point, we decided to redesign the database taking into account the present-day information requirements of water resource managers and current sampling and data collection procedures. Drawing heavily on our

experience with the SYSTEM 2000 DBMS and it's inadequacies, we surveyed Water Quality Branch staff to determine what information should be stored and how it should be used. A number of criteria were established, as follows:

1. All information relating to characteristics or geographic allocation of the sampling site would be stored in the stations table.

2. Information on the water type or sample media would be stored in a samples table. On the existing database, this information is part of the station number.

3. The station name must be meaningful, such as Ottawa River at Lemieux Island or Black Lake at Centre.

4. There must be a unique sample identifier or sample number. The existing database does not have this feature.

5. The variable (parameter) code will relate to the variable only and will not reference information on the analytical or measurement method. A method code is being established for this purpose. The system itself will keep track of valid combinations of variable and method codes. This will greatly reduce the number of codes in the dictionary.

6. Where samples are split and sent to different laboratories, it is important to keep track of all the parts and know which variables were measured in which laboratories.

7. The database must be able to keep track of spatial and temporal composite samples and relate the individual sample numbers to the composite sample number.

Once all the criteria were established, we looked at possible database organizations. Water quality data tend to fit the hierarchical data structure very well (i.e. three levels, stations, samples, variables). The task was to develop a relational model for these data. The conversion of the existing data necessitated that the water chemistry structures be addressed first.

We considered the typical water quality data-collection process. First a water resource officer travels to a location on a water body (the sampling site). Secondly, samples are collected at the site. These could be water, sediment, or biological samples. Thirdly, measurements are made on these samples, usually at a laboratory. Based on this process we decided to design three tables "STATIONS", "SAMPLES", and "MEASUREMENTS".

The "STATIONS" Table

The "STATIONS" table (TABLE 2) contains all the information relative to the location of the site such as station_no, station_name, etc. The coordinates of the site location can be stored as latitude and longitude, or as UTMs (Universal Transmercator Grid). The station_name must be meaningful (i.e. Ottawa River at Lemieux Island). The active_indicator field which can have values of Y or N will eventually be used for archiving stations that have not been sampled for ten years or more.

The "SAMPLES" Table

The "SAMPLES" table (TABLE 3) is where the existing and new databases diverge. Much more useful information relating to the sample can be stored in the new relational database. The most important field is the sample_no. This field, which is alphanumeric, must be unique for all samples on the database. Information on the sample media, the type of sample (i.e. discreet, integrated, blank, etc.) and how the sample was collected is coded and stored in this table. The project_no is a number which identifies the project for which the sample was collected. Where samples are part of a composite sample, the composite sample number can also be stored. Descriptions of all the codes are found in other tables.

The "MEASUREMENTS", "VARIABLES" and "VALID_MTHD_VAR" Tables

When trying to design the "MEASUREMENTS" table (TABLE 4), problems arose with the variables and

TABLE 1: SYSTEM 2000 DATABASE SCHEMA

```
DATA BASE NAME IS NAQPAC
DEFINITION NUMBER      6
DATA BASE CYCLE      31552
    1* STATION (CHAR X(12))%
    2* WATER TYPE (CHAR XX)%
    3* PROVINCE (CHAR XX)%
    4* BASINS (CHAR XXXX)%
    5* LAT (DECIMAL NUMBER 99.9(5))%
    6* LONG (DECIMAL NUMBER 999.9(5))%
    7* PRECLL (NON-KEY CHAR X)%
    8* NARRATIVE (NON-KEY TEXT X(200))%
    9* REFERENCE STN (NON-KEY CHAR X(12))%
   10* AVER DEPTH (NON-KEY DECIMAL NUMBER 9999.9)%
   11* DIST FROM REF STN (NON-KEY DECIMAL NUMBER 9999.99)%
   12* WSC STN (NON-KEY INTEGER NUMBER 999)%
   13* LAST DATE UPDATED (DATE)%
   14* XREF STN (NON-KEY CHAR X(6))%
  100* SAMPLES (RECORD)%
    101* SDATE (DATE IN 100)%
    102* SMONTH (NON-KEY INTEGER NUMBER 99 IN 100)%
    103* STIME (NON-KEY INTEGER NUMBER 9999 IN 100)%
    104* SDATETO (NON-KEY DATE IN 100)%
    105* STIMETO (NON-KEY INTEGER NUMBER 9999 IN 100)%
    106* TIME ZONE (NON-KEY CHAR XXX IN 100)%
    107* PRECTIME (NON-KEY CHAR X IN 100)%
    108* FREQ (NON-KEY CHAR XX IN 100)%
    109* SAMPLE NUMBER (NON-KEY CHAR X(7) IN 100)%
    110* LAB CODE (CHAR XX IN 100)%
    111* PROJECT (INTEGER NUMBER 9999 IN 100)%
    112* COMMENTS (NON-KEY CHAR X(23) IN 100)%
    113* DEPTH (NON-KEY DECIMAL NUMBER 9999.9 IN 100)%
    200* PARAMETER VALUES (RECORD IN 100)%
      201* PARM CODE (CHAR X(6) IN 200)%
      202* FLAG (NON-KEY CHAR XX IN 200)%
      203* VALUE (NON-KEY DECIMAL NUMBER 9(6),9(5) IN 200)%
```

TABLE 2: STATIONS

NAME	NULL?	TYPE
STATION_ID		CHAR (2)
STATION_NO	NOT NULL	CHAR (10)
STATION_NAME	NOT NULL	CHAR (50)
STATION_DESC		CHAR (240)
OTHER_STATION_NO		CHAR (40)
LATITUDE		CHAR (9)
LONGITUDE		CHAR (10)
UTM_ZONE		NUMBER (2)
UTM_EAST		NUMBER (8,1)
UTM_NORTH		NUMBER (7,1)
AVG_DEPTH		NUMBER (6,1)
WSC_NO		NUMBER (3)
ACTIVE_INDICATOR		CHAR (1)
CREATION_DATE		DATE

TABLE 3: SAMPLES

NAME	NULL?	TYPE
SAMPLE_NO	NOT NULL	CHAR (10)
STATION_NO	NOT NULL	CHAR (10)
PROJECT_NO		CHAR (5)
AGENCY_CODE		CHAR (3)
SAMPLE_TIME	NOT NULL	DATE
SAMPLE_END_TIME		DATE
SAMPLE_DEPTH		NUMBER (6,1)
TIME_ZONE	NOT NULL	CHAR (3)
MEDIA_CODE		CHAR (10)
CLASS_CODE		CHAR (10)
COLLECTION_CODE		CHAR (15)
X_REF_SAMPLE_NO		CHAR (20)
COMP_SAMPLE_NO		CHAR (9)
E_COMMENT		CHAR (240)
F_COMMENT		CHAR (240)
UPDATE DATE		DATE

TABLE 4: MEASUREMENTS

NAME	NULL?	TYPE
SAMPLE_NO	NOT NULL	CHAR (9)
LAB_CODE	NOT NULL	CHAR (10) null allowed for initial load
LAB_SAMPLE_NO	NOT NULL	CHAR (9)
VMV_CODE	NOT NULL	NUMBER (6) null allowed for initial load
VARIABLE_CODE	NOT NULL	CHAR (20)
SAMPLE_DETECT_LIMIT		NUMBER (12,5)
FLAG		CHAR (1)
VALUE		NUMBER (12,5)
OBSERVATION		CHAR (20)
MEAS_DATE		DATE
OLD_PARA_CODE		NUMBER (6) X-ref for initial load

TABLE 5: VARIABLES

NAME	NULL?	TYPE
VARIABLE_NO	NOT NULL	CHAR (20)
VARIABLE_NAME	NOT NULL	CHAR (50)
VARIABLE_GROUP		CHAR (50)
OTHER_NAME		NUMBER (50)

analytical methods, and how to handle valid combinations of these.

On the existing system, information on the variables, units, and analytical methods are all contained within the parameter code. As explained earlier the parameter code is a five-digit number, the first two digits being the atomic number of the element. In the early days, this was adequate and worked well; however, the proliferation of organic contaminants and the need to store biological variables has made the system obsolete. Everytime the laboratory improved a method for a class of organic contaminants, we had to add 50 or more new parameter codes. This became very inefficient, especially when trying to retrieve data.

The new system is quite different. There is a "VARIABLES" table (TABLE 5) which stores the lists of variable codes, names, and variable groups for which information is stored on the database. The new variable-coding system uses the chemical abstract registry number for all the organic compouds and a mnemonic alphanumeric system for the physical, inorganic, and biological variables.

The "VALID_MTHD_VAR" table (TABLE 6) relates variables to the measurement method codes and stores information on detection limits, units, and an expected upper limit (used for flagging unexpected high values on data input). For each of these combinations, the computer will assign a VMV code (valid method variable). This code is then stored in the "MEASUREMENTS" table to relate these fields to the data. In effect, it plays a similar role to the existing NAQUADAT parameter code.

The "MEASUREMENTS" table stores the data. It is related to the "SAMPLES" table by the sample_no. In the early days, the analysis of the samples was usually completed by one laboratory. Today samples are often split and sent to different laboratories since each laboratory has different capabilities. For example, a smaller regional laboratory may analyse samples for variables requiring immediate analysis or requiring less sophisticated methods, whereas variables requiring expensive instrumentation may be

sent to a central laboratory. In any case it is important to know which variables were measured at which laboratory and to be able to merge all these results under the one original sample number. The lab_code and lab_sample_no allow this to be easily accomplished.

The data can be stored as either a numeric value or as an alphanumeric observation. On the existing database, data for any variable can be stored in a variety of units. On the new database, all data for one variable will be stored in one set of units. Conversion will be performed on input if required.

On completion of these tables, entity-relationship modelling was performed to the third normal level. This resulted in the final database design, as shown in FIGURE 1.

It should be mentioned here that we have not yet addressed toxicity data from the various toxicity tests that are currently in use. This data will eventually be included on the database.

BIOLOGICAL DATA STORAGE

Design of the biological data storage focussed on the variety of biological data types and how the database structure (outlined under DATABASE DESIGN) could be used. As a result of this study, three additional tables will be added to the database to allow a full description of the biological samples. These tables are "BIO_ITEMS", "TISSUE_ITEMS", and "TAXON_CODES".

The table "BIO_ITEMS" (TABLE 7) contains information about a specific biological item, such as taxonomic and age/sex classifications, from the sample on which the measurement was made. The table "TISSUE_ITEMS" (TABLE 8) contains information about a specific piece of tissue.

Two fields, one from each table, will be added to the "MEASUREMENTS" table to join these tables. A media code in the "SAMPLES" table will indicate that the sample is biological and additional information is available. The field taxon_code in the "BIO_ITEMS" table allows joining to the

TABLE 6: VALID_MTHD_VAR

NAME	NULL?	TYPE
VMD_CODE	NOT NULL	NUMBER (6)
METHOD_CODE	NOT NULL	CHAR (20)
VARIABLE_CODE	NOT NULL	CHAR (20)
UNIT	NOT NULL	CHAR (10)
METHOD_DETECT_ LIMIT		NUMBER (8,3) null allowed for initial load
UPPER_LIMIT		NUMBER (8,3)
OLD_PARM_CODE		CHAR (6)
CREATION_DATE		DATE

TABLE 7: BIO_ITEMS

NAME	NULL?	TYPE
SAMPLE_NO	NOT NULL	CHAR (9)
BIO_ITEM_NO	NOT NULL	NUMBER (6)
TAXON_CODE	NOT NULL	CHAR (10)
LIFE_STAGE_CODE		CHAR (10)
SEX		CHAR (1)
AGE		CHAR (8)
AGE_MTHD_CODE		CHAR (10)
PRESERVATION_ CODE		CHAR (10)
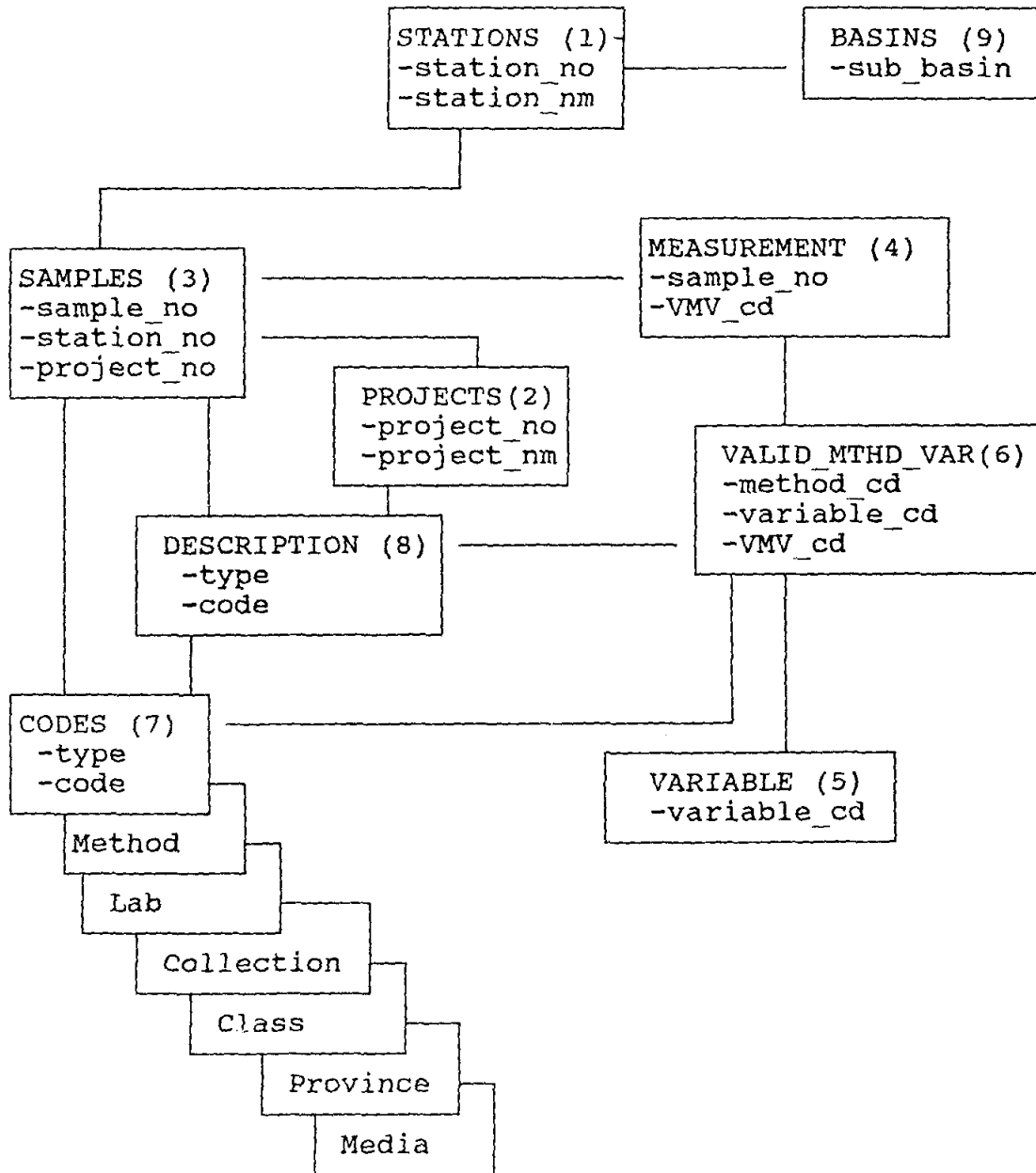
TABLE 8: TISSUE_ITEMS

NAME	NULL?	TYPE
SAMPLE_NO	NOT NULL	CHAR (9)
BIO_ITEM_NO	NOT NULL	NUMBER (6)
TISSUE_ITEM_NO	NOT NULL	NUMBER (6)
TISSUE_TYPE_CODE	NOT NULL	CHAR (10)
PRESERVATION_ CODE		CHAR (10)

TABLE 9: TAXON_CODES

NAME	NULL?	TYPE
TAXON_CODE	NOT NULL	CHAR (10)
GENUS		CHAR (40)
SPECIES		CHAR (40)
COMMON_E_NAME		CHAR (60)
COMMON_F_NAME		CHAR (60)
SUPERIOR_TAXON	NOT NULL	CHAR (40)
ALT_SUPERIOR_ TAXON		CHAR (40)

"TAXON_CODES" table (TABLE 9) which stores the taxonomic information.

STORAGE and RETRIEVAL

Information will be stored and retrieved either through batch processing or by using screens. A series of menus will be set up to guide a user to the information he or she is searching for. This information can be displayed on the screen in user views or by hard copy. Data in machine-readable format will also be available. The level of privileges assigned to any user will depend on their capability and availability of hardware and software.

CONCLUSION

The new NAQUADAT database will be a major improvement over the existing system. It will provide a facility for storing many different types of water quality information. It will provide the flexibility and user-friendliness required by today's water resource managers.

One type of data that has not yet been addressed is toxicity data from the various toxicity tests that are currently in use.

REFERENCES

Demayo A, and E Hunt, 1975, "NAQUADAT Users Manual", Inland Waters Directorate, Water Quality Branch, Ottawa,Canada, K1A OH3.

Demayo A, M Lamb, and S Whitlow, August 1986, "NAQUADAT in the 1980s", Water Quality Branch, Inland Waters Directorate, Conservation and Protection, Environment Canada, Ottawa, Canada, K1A OH3.

OVERVIEW OF WATER QUALITY INFORMATION SYSTEMS FROM A STEERING COMMITTEE PERSPECTIVE

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INTRODUCTION

The U.S. Environmental Protection Agency (EPA) Office of Water (OW) has developed and operates several data management systems that provide water quality planners and regulatory decision makers with information needed to promulgate and enforce water quality regulations that protect the waters of the United States. Examples of key Federal data systems maintained and utilized by EPA include STORET (for storage and retrieval of water quality and other data), the Reach File (for stream characteristics organized in hydrological order), and the Waterbody System (for surface water quality compliance status and trends). These and other systems have been developed, managed, maintained, operated, and up-graded by different Offices within OW. These activities are usually carried out independently of other OW offices and data management systems. Recently, however, changes in the way the Agency (EPA) conducts its business -- specifically, technological, programmatic, statutory, and policy modifications -- have prompted a need for changes in the manner in which these systems are operated and used.

The Office of Water recognized the need for a new data system management approach in its 1987 report entitled Surface Water Monitoring: A Framework for Change. Commonly known as SWMS (the Surface Water Monitoring Study), the report identifies, among others, the following obstacles to providing water quality managers with the information required to make effective, environmentally sound decisions:

Water quality managers are skeptical about the quality and usefulness of data from unidentified sources. Therefore, these data are often not used to develop plans, set priorities, or make operational decisions.

EPA's water-related data bases are difficult to access and use.

EPA and State water quality managers and staff are unaware of the availability of potentially useful data which can be accessed through Federal (including EPA), State, and other data systems.

The SWMS report makes two major recommendations for overcoming these obstacles:

1. Improve EPA and State users' knowledge of sources and applications for existing water-related data.

2. Establish centralized coordination of all EPA efforts to integrate water-related data.

In response to the above SWMS report recommendations, OW Office Directors authorized the formation of the Steering Committee for Water Quality Data Systems (the Steering Committee). The purpose of the Steering Committee is to 1) guide the continued development and management of the STORET system, 2) oversee water quality data systems that support OW programs, and 3) ensure that Agency and State water-related data management needs are met.

This paper describes the Steering Committee, its structure, its operation, and its commitment to communication, cooperation, and consensus-building. Also, the paper focuses on Steering Committee recommendations, the "priority" water-related

data systems it has identified, and the results of the Steering Committee's efforts to date.

STEERING COMMITTEE STRUCTURE AND FUNCTION

The structure and function of the Steering Committee for Water Quality Data Systems reflects the OW's commitment to inter-Office cooperation, communication, and consensus-building as means for improving OW data systems.

Steering Committee Structure

Six of the seven Office of Water (OW) Offices are represented on the Steering Committee: the Office of Ground Water Protection (OGWP), the Office of Water Regulations and Standards (OWRS), the Office of Water Enforcement and Permits (OWEP), the Office of Drinking Water (ODW), the Office of Municipal Pollution Control (OMPC), and the Office of Marine and Estuarine Protection (OMEP). Each of the ten EPA Region offices is also represented on the Steering Committee, as are State agencies and the EPA's Office of Information Resources Management (OIRM). (OIRM is the EPA office respon- sible for technical and management direction in data processing.) See Figure 1. Steering Committee representatives are typically managers who can speak authoritatively for a sponsoring EPA Office, program, data system, or user population. See Table 1. This representation approach promotes communi- cation and cooperation between system managers, program leadership, and OW executives by bringing key personnel together for discussions of issues related to water quality data and its management.

The Steering Committee is comprised of two fundamental structural components: Steering Committee members, and General Meeting attendees. There are 13 voting Steering Committee members; one each from 5 of the EPA OW Headquarters Offices, one each from 6 Region offices, and one each from a State and OIRM. Although ideas and input from many managers, decision-makers, technical advisors, and system users are actively sought, OW Office Directors limited the size of the voting membership to maximize effectiveness of the Steering Committee.

Other groups are represented by the second structural component of the Steering Committee, the General Meeting attendee. Once or twice each year, the Steering Committee conducts a General Meeting for Steering Committee members and attendees. Meeting attendees represent Headquarters, Region, and State organizations which have an interest in water-related data management systems. Although they do not vote directly on Steering Committee actions, attendees assist in setting agenda, considering issues, and participating in one of the Steering Committee's three work groups.

The three work groups, established in the Steering Committee functional statement, include the Communications Workgroup, the Technical Workgroup, and the Policy and Management Workgroup. The Communica- tions Workgroup considers and recommends means by which water-related data systems users and managers can be kept informed about data and systems. This includes communications regarding Steering Committee discussions, recommendations, and activities. The Technical Workgroup focuses on system enhancements and applications, feasibility of new technologies, and assessment of existing systems. Finally, the Policy and Management Workgroup deals with the overall direction and management of OW data systems and data use.

Steering Committee members participate with and are -- in part -- accountable to General Meeting attendees. Attendees receive minutes of Steering Committee member meetings. This assures that attendees are aware of Steering Committee decisions and issues under consideration. Attendees provide valuable feedback to members. They communicate concerns, ideas, and decisions between the Steering Committee and the organizations which they represent. The interaction between Steering Committee members and attendees facilitates consensus-building among those with an interest in water-related data management systems.

Figure 1.

Steering Committee Representation Structure
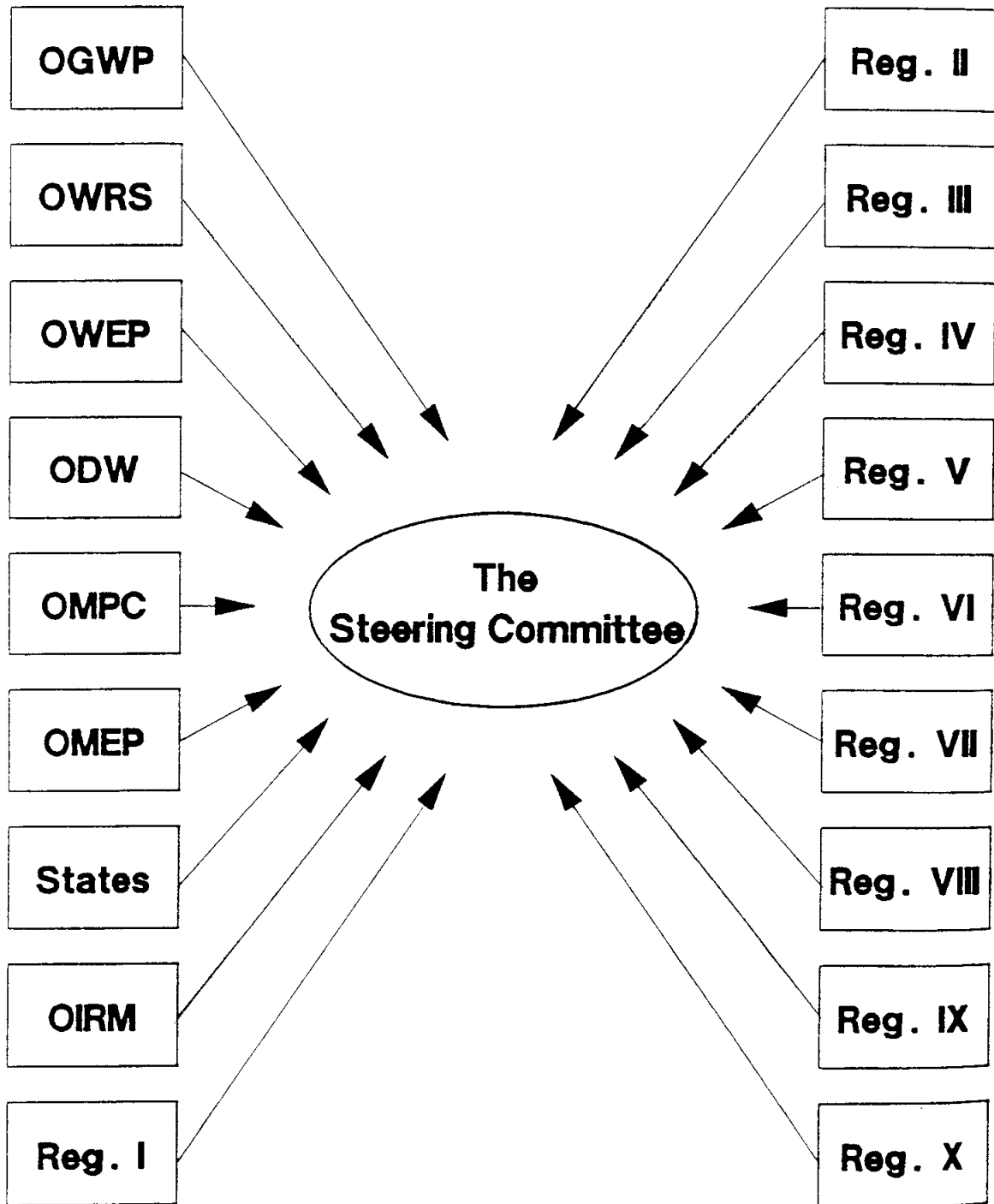
Table 1

OW Priority Data Systems Represented on the
Steering Committee for Water Quality Data Systems

Responsible Office	System	Function
OWRS/OIRM	BIOS	Aquatic Organism Data Storage and Analysis
OWRS	REACH	Hydrologic Identification of Surface Water Features
OIRM/OWRS	STORET	Storage and Retrieval of Environmental Information for Surface and Ground Waters
OWRS	WBS	Stressed Waters Lists and Reporting Requirements for Clean Water Act Section 305(b)
OWEP	PCS	Permit, Compliance, and Enforcement Information
OMPC	NEEDS	Estimations of Investments Required for Construction of Waste Water Treatment Facilities
OMPC	GICS	Waste Water Treatment Facility Construction Project Tracking
OMEP	ODES	Marine Biological and Water Quality Monitoring, Permit/Compliance Data
OWRS	DWS	Surface Water Supply Data
ODW	FRDS	Public Waters Supplies Program Data
OWRS/OIRM	GAGE	USGS Stream Gaging Location Information
OWRS/OIRM	IFD	Industrial and Municipal Point Source Discharge Information

Steering Committee Function

Shortly after the Steering Committee formed, members developed a functional statement which was subsequently approved by the Office of Water Office Directors (ODs). In the approved functional statement, ODs gave the Steering Committee the responsibility of providing guidance on policy, management, and general technical issues. This guidance is in the form of recommendations to OW Office Directors and the OW Senior Information Resources Management Officer (SIRMO). Office of Water ODs, who established the Steering Committee and authorize its activities, must concur on recommended actions. The Steering Committee is also responsible for managing the execution of its recommended actions and reporting progress and task completion to the ODs.

INITIAL ACTIONS

The Steering Committee's first actions addressed three immediate needs: 1) The Steering Committee agreed on member and attendee roles and responsibilities and began the development of a functional statement for OD approval; 2) Program managers within the Steering Committee received the support of the Steering Committee to conduct mission need and user requirements studies for the addition of toxicity and tissue residue components to BIOS; and 3) The Steering Committee sought to ensure communication between members and attendees by establishing a process for distributing meeting minutes and publishing activity summaries in Agency reports and newsletters.

RECOMMENDATION DEVELOPMENT PROCESS

The primary process by which the Steering Committee effects change is recommending actions to Office Directors and the OW SIRMO. On February 14, 1989 the Steering Committee delivered its first recommendations to the ODs. The recommendation memorandum represented the culmination of a process that began in May of 1988 at the Steering Committee General Meeting held in Crystal City, Virginia (see Figure 2). This meeting of members and attendees featured work group discussion sessions and assembly meetings of the entire group. The primary outcome of this meeting was a list of 30 issues to be considered for Steering Committee action. Members agreed to review the 30 statements and prepare for a prioritization vote at the next Steering Committee meeting.

That meeting was conducted in conjunction with the June 2-3 National Symposium on Water Quality Assessment in Annapolis, Maryland. On June 2, 1988, Steering Committee members caucused with 13 representatives from State agencies to introduce the Steering Committee, review the 30 considered issue items, and solicit comments.

On the following day, Steering Committee members voted to focus further consideration on nine of the 30 preliminary subject areas. Members then agreed to develop an issue paper for each of the nine topics. Completed issue papers were discussed during telephone conference calls (June 26, July 21, September 1, October 13, November 17, and December 9). Recom- mendations from each of the issue papers were consolidated into a comprehensive paper entitled "Steering Committee for Water Quality Data Systems Recommenda- tions for Committee Actions" (November 8, 1988). This paper described ten general and ten specific action recommendations.

A final round of Steering Committee voting resulted in the recommendations for the February, 1989 Steering Committee memorandum to the OW Office Directors. By mid-March, 1989, the Office of Water Directors concurred with the Steering Committee recommendations and com- mented on priorities. Efforts are now underway to carry out the actions approved by the OW Office Directors.

The approved recommendations fall into two general categories: 1) Data Sharing and System Integration/Compatibility, and 2) User Training and System Accessibility. The first category reflects the Steering Committee's

Figure 2

MILESTONES IN STEERING COMMITTEE ACTIVITIES

1988 MAY	JUNE	JULY	AUG	SEPT	OCT	NOV	DEC	1989 JAN	FEB	MARCH	APRIL	MAY	JUNE	JULY	AUG	SEPT	OCT

■ General Meeting (Crystal City)

  ■ State Caucus in Annapolis

■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■ ■
Monthly Telephone Conference Calls

■ Combined Position Paper on Recommendations

■ Recommendations Delivered to Office Directors

■ OD Concurrence

■ Start of Integration Study

■ Forums Start

concern with the apparent boundaries that exist between independently developed OW data management systems. The Steering Committee members, in agreement with the authors of the SWMS report, believe that opportunities for making better decisions are being overlooked because data from the various systems cannot be easily integrated. The recommendations which fall under the second category communicate the Steering Committee's concern that access to valuable data is difficult or lacking. Water quality managers and analysts often are not aware of the sources and types of data that are available, nor are they knowledgeable about how to operate the systems within which these data reside. Those who are familiar with the data and data management systems, are often discouraged because hardware is inconveniently situated, queries require sophisticated understanding of search terms and syntax, log-on and security requirements are cumbersome, and flexible user-friendly applications (report generation packages, graphics tools, statistical analyses) are not always available.

In order to address these two major areas of concern, the Steering Committee has developed specific recommendations for action.

RECOMMENDATIONS

Priority Data Systems

The Steering Committee recommended that it limit the scope of its considerations to the "Priority OW Data Systems." These systems are discussed in detail below.

BIOS

The **Field Survey Component** of BIOS is a national biological information management system which processes data on the distribution, abundance, and physical condition of aquatic organisms, and descriptions of their habitats. Its link to STORET allows the association of biological data with water chemistry data. The system offers analytical tools which facilitate consistent assessments of water quality and biological integrity. All data in BIOS are associated with sample location identifiers. Sampling locations, i.e., stations, are identified within the system using geographic descriptors including latitude-

longitude coordinates, and drainage basin, State, county, and ecoregion designations. Individual field surveys are also uniquely identified. Habitats are described by substrate type, embeddedness, streambank stability, and canopy type.

Requirements studies for the addition of toxicity testing and tissue residue components of BIOS have been recom- mended by the Steering Committee and are currently in progress. (For more detailed BIOS information, contact Phil Linden- struth, (202) 382-7220 or (800) 424-9067.)

DWS

The **Drinking Water Supply File** contains data on U.S. surface water supplies, including locations of utilities, intakes and sources, and the hydrological cataloging unit numbers and reach numbers of utility receiving waters. The data base contains data on 824 utilities serving communities with populations greater than 25,000, and 6,840 utilities serving communities with populations less than 25,000. (For more detailed DWS information, contact Phill Taylor, (202) 382-7046.)

FRDS

The **Federal Reporting Data System** contains descriptive compliance information about public water supply systems. Individual facilities report periodic compliance events, such as violations of MCLs for particular chemicals, which are tracked and reported by FRDS. (For more detailed FRDS information, contact A.W. Marks, (202) 382-5515.)

GAGE

The **Stream Gage/Flow File** contains information from approximately 36,000 stream gaging locations throughout the United States. Location of gaging stations, types of data collected, frequency of data collection, collecting agency, and mean and annual flow and 7Q10 low flow are available. The Stream Gage/Flow File provides a common repository for gage information and supports activities such as water quality studies, waste load allocation, dilution studies, and water

treatment assessments. This file may also contain estimated flow and velocity information for mean and low flow conditions of stream segments. (For more detailed GAGE information, contact Phill Taylor, (202) 382-7046.)

GICS

The **Grants Information Control System** is the primary source of information pertaining to Federal (EPA) construction grants projects for municipal waste water treatment facilities. (For more detailed GICS information, contact Janie Latta, (202) 382-5831.)

MIFD

The **Municipal/Industrial Facilities Discharge File**, containing over 119,000 NPDES facilities, was designed and implemented for the purpose of providing a comprehensive data base of industrial and municipal point source dischargers to U.S. surface waters. The data base includes general information about each facility including: discharge and location information for direct and indirect point source discharges, standard industrial classification (SIC) codes, and categorization of process and discharge type. (For more detailed IFD information, contact Phill Taylor, (202) 382-7046.)

NEEDS

The **Needs Survey File** comprises data, analytical tools, and reporting utilities required for estimation of funds needed for the construction of municipal waste water treatment facilities. This system supports activities required under §205(a) and §516(b)(1) of the Clean Water Act. (For more detailed NEEDS information, contact Joyce Hudson, (202) 382-7251.)

ODES

The **Ocean Data Evaluation System** is a data management and analysis system that supports regulatory decision-making associated with marine monitoring programs. It was originally designed to support EPA's 301(h) Program, but has since been adapted for use in other marine monitoring programs. ODES

is comprised of two main components, the data base files (containing water quality, aquatic organism, and permit/compliance data) and the analytical tools (for statistical analyses, temporal and spatial plots, data tabulation, graphical design). (For more detailed ODES information, contact Robert King, (202) 475-7119.)

PCS

EPA requires NPDES permit holders to monitor the composition of their waste water effluents and report results regularly to the permitting agency (State or EPA Regional Office) via Discharge Monitoring Reports (DMRs). The regulated community submits approximately 800,000 DMRs per year. DMR data from major sources and significant minor sources are entered into the **Permit Compliance System** for automated comparison against permit limitations. (For more detailed PCS information, contact Dela Ng, (202) 475-8323.)

REACH

The **Reach File** is a digital data base containing streams, lakes, reservoirs, and estuaries which have been divided into unique segments called "reaches." (Reaches may also be divided into subreaches.) Each of the 68,000 reaches included in the Reach File is identified by an unique eleven-digit number. The data available from the file include stream and open-water names, stream and shoreline traces, and mileage information. Reach inter-relationships are organized in a manner which allows upstream and downstream analysis of river and open water conditions by scanning other data files for "reach-indexed" information. The Reach File is the foundation of EPA's ability to integrate data from other data bases. (For more detailed REACH information, contact Phill Taylor, (202) 382-7046.)

STORET

STORET is a computerized data system maintained by EPA for the storage and retrieval of environmental data pertaining to the quality of the nation's waterways. STORET is comprised of three systems.

These systems, the Water Quality system, the Biological Data system, and the Stream Flow system, access many data files and hence, various types of information. These files are: the Water Quality file, the Reach File, Stream Gage/Flow file, Pollution Caused Fish Kill Report file, Drinking Water Supply file, City/County Geographic file, and the BIOS Field Survey and Taxonomy files. Report retrieval, statistical analyses and geographic plotting procedures are available via STORET (in batch and conversational modes) for all users of the EPA National Computing Center (NCC) in RTP, North Carolina. (For more detailed STORET information, contact Phil Lindenstruth, (202) 382-7220 or (800) 424-9067.)

WBS

The **Waterbody System** is an inventory of waterbodies which have been assessed for water quality. The WBS serves as the basis for the biennial 305(b) report to Congress. It also serves as the mechanism for fulfilling the following Water Quality Act of 1987 requirements: listing of waters requiring control strategies; identification and characterization of publicly owned lakes; and identification and characterization of waters affected by non-point sources. The WBS has approximately 25 data elements for information on the identity and description of the waterbody, the designated uses, the water quality status, status determination rationale, pollution sources, and planned activities. The Checklist File which contains information on monitoring and wasteload allocation planned activities from the State grant applications will be merged into this system. (For more detailed WBS information, contact Meg Kerr, (202) 382-7056.)

RECOMMENDATIONS

The Steering Committee has recommended that the following actions receive highest priority attention for near-term completion:

Data Sharing and System Integration Study

The Steering Committee recommended a study to assess each priority system's potential for inter-system data sharing and integration.

The Steering Committee determined that a rational, systematic approach to promoting and developing mechanisms for inter-system sharing and integration of information cannot be developed without an assessment of the existing data management systems. The study to assess these potential capabilities will minimally address the criteria listed below:

1) Does the system contain minimum data sets/data fields which facilitate inter-system linking of data records?

2) Does the system provide a means to readily access and display/overlay data from other systems?

3) Does the system contain a latitude/longitude coordinate set or another coordinate set that would allow data integration via a Geographic Information System?

4) Does the system provide a means for easily downloading and uploading data via PC?

5) Can system security measures be modified to encourage data sharing and exchange without risking data loss/corruption?

6) Are data evaluated during collection and data entry to determine their quality?

7) Are on-line reports available that address data quality and factors affecting interpretation?

Results of this study will be in the form of a specific set of recommended enhancements and/or activities for each priority data system listed above.

The Steering Committee recommended that individual system and program managers be responsible for implementing the enhancements and/or activities recommended in the study report. The Steering Committee will report to OW Office Directors on progress towards implementing the study recommendations.

Enhancements to The Reach File

The Steering Committee recommended the following enhancements to the Reach File:

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1. *Completely install and maintain the 1988 Reach File (RF2).* This installation will effectively double the existing number of reaches (68,000) contained in the Reach File.

2. Complete the assembly of USGS DLG (digital line graph) segments into Reach cataloging units and overlay onto the 1988 Reach File (RF2).

   The 1988 Reach File (RF2) contains detailed hydrologic structure information such as stream name, reach connectivity, and hydrologic routing data. The latitude/longitude coordinate data ("traces") in RF2, consist only of coordinates for the endpoints of each reach segment and points spaced approximately every five miles in between. The USGS DLG (digital line graph) database contains very detailed coordinate line trace information, but very little hydrologic structure information. By incorporating DLG coordinates into RF2, the Reach File (RF3) will contain full hydrologic connectivity information and detailed trace coordinates. These detailed coordinates will provide several benefits including accurate stream milage estimates and the ability to produce high-quality Reach File maps. Further, the detailed coordinate traces will provide greatly enhanced capabilities for indexing other data to the Reach File. These include data from STORET, GAGE, IFD, and PCS.

3. Add surface area segmentation and finite element modeling capabilities for estuaries and open waters. This significant system enhancement will give data quality managers and analysts the ability to readily represent lakes and estuaries (for purposes of modeling and spatial characterization) as integrated parts of a complete watershed system. The effects of adjustments to upstream discharge levels could be quickly portrayed for use in a variety of regulatory scenarios.

4. Categorize reach segments into ephemeral and perennial flow groups. This information can be incorporated from DLG files.

5. Add reach files for the Pacific Islands, Puerto Rico, Alaska, and Hawaii. Because reach files for these areas do not currently exist and because DLG data of appropriate resolution are not available, a preliminary effort to clarify goals, assess data availability, consider project options, and refine an approach should be undertaken.

6. Add PC digitizing capabilities.

7. Add capabilities for uploading and downloading database files between the mainframe and PCs, and for "live" access to mainframe data via the PC Reach File.

Regional Forums for Information Transfer

The Steering Committee recommended that information transfer Forums be conducted in each of the ten EPA Regions. These forums should be designed to demonstrate potential applications of recent enhancements to the priority data systems and to solicit feedback from those who attend the Forums.

The Forums should contribute towards meeting several of the critical needs identified in the SWMS report:

1) Water-quality managers and analysts will be formally introduced to most of the priority data systems and the data available on each system.

2) Users will be given the opportunity to operate systems of interest. This is particularly important for system access problem resolution. Users will learn which hardware are available, how to log-on, and whom to contact for assistance.

3) Users will be introduced to systems applications. Questions about how priority data systems can assist in day-to-day decision-making activities will be addressed. Specific solutions will be demonstrated and practiced under supervision of experienced users/trainers.

4) Users will have an opportunity to demonstrate their system applications for

Steering Committee representatives. This will allow the transfer of information to other Regions and States.

5) Users will be able to communicate their needs and system requirements ideas in the form of feedback to those responsible for maintaining and enhancing the priority systems.

Menu-Driven Data Entry and Retrieval Software for STORET

OIRM, with OWRS and OGWP, is managing efforts to simplify the retrieval process for STORET's Water Quality System (WQS). This project will result in the full implementation of eleven WQS data displays which will prompt users for retrieval request input. The software will analyze user query information and submit the appropriate request to the WQS. Users will not be required to learn the STORET retrieval language.

Menu-driven station storage input software is also being developed. This software simplifies the data input process required for positioning and classifying monitoring station locations. This software will eliminate the need for users to know the command language for the system in which STORET operates.

The Steering Committee recommends completion of these projects to increase the ease with which STORET can be used.

PROGRESS ON RECOMMENDED ACTIONS

The Steering Committee has selected and funded a contractor to conduct the Data Sharing and System Integration Study. Work will commence soon. A report to the Steering Committee should be completed by March, 1990.

The 1988 Reach File (RF2) has been completely installed. Also, PC digitizing and file uploading/downloading capabilities are available for use by the Waterbody System. DLG files have been converted with latitude/longitude coordinates. Edge matching and assignment to Reach cataloging units are complete. The DLG overlays for EPA Regions IV and V will be completed by January, 1990. Specific plans for adding new reach files (Hawaii, Alaska, etc.), adding finite element spatial representation for estuaries, and adding ephemeral/perennial classifications will be discussed with the Regions and States at the Regional Forums.

The Regional Forums will begin on June 13, 1989. Forums will be conducted in eight of the ten EPA Regions during this fiscal year (ending September 30, 1989). Completion of the final Forum is scheduled for FY '90. Feedback from the initial Forums will be addressed at the next Steering Committee General Meeting to be held during the first quarter of Fiscal Year 1990 in Washington, DC.

Software development for the first five STORET retrieval screens was completed in October, 1988. The final six retrieval screens should be completed before January, 1990. Also, the menu driven station storage software is scheduled for completion by September 30, 1989.

SUMMARY

The accomplishments which have been brought about by the efforts of the Steering Committee for Water Quality Data Systems support the views of the OW Office Directors and the authors of the SWMS report that cooperation, communication, and consensus-building between managers and users of water-related data systems will promote progress towards providing water quality managers with the information needed to make more effective and environmentally sound decisions.

The Steering Committee has been fully active since May, 1988. A list of members and attendees is provided in Table 2. Steering Committee members and attendees are available to provide information on priority OW data systems and to consider additional recommendations for improving data quality and OW data management

Table 2

STEERING COMMITTEE MEMBERS

NAME	OFFICE	FTS[*] PHONE	NON FTS
Dee, Norbert	OGWP	FTS-382-7077	(202)-382
Lindenstruth, Phil	OIRM	FTS-382-7220	(202)-382
King, Robert	OMEP	FTS-475-7119	(202)-475
Ehrensberger, Kathleen	OMPC	FTS-382-5386	(202)-382
Martin, Steve	OWEP	FTS-475-8313	(202)-475
Myers, Carl	OWRS	FTS-382-7040	(202)-382
Manfredonia, Ron	Reg. I	FTS-835-3531	(617)-565
Malleck, John	Reg. II	FTS-264-5635	(212)-264
Ehorn, Doug	Reg. V	FTS-886-0243	(312)-886
Svoboda, Larry	Reg. VIII	FTS-776-5102	(303)-236
Kuhlman, Catherine	Reg. IX	FTS-454-8312	(415)-974
Eusebio, Ben	Reg. X	FTS-399-0422	(206)-442
Haire, Mike	St. of MD		(301)-631-3680

STEERING COMMITTEE ATTENDEES

NAME	OFFICE	FTS PHONE	NON FTS
Conger, Sam	NDPD/RTP	FTS-629-0613	(919)-541
Linthurst, Rick	OADEMQA	FTS-629-4048	(919)-541
Zenon, Michele	OGWP	FTS-382-7077	(202)-382
Miller, Jerry	OIRM	FTS-382-2374	(202)-382
Tasker, Connie	OIRM	FTS-475-8675	(202)-475
Braswell, Sandy	OMPC	FTS-382-7251	(202)-382
Devonald, Kim	OPPE	FTS-475-8214	(202)-475
Blakeslee, Mary	OW	FTS-382-7818	(202)-382
Widdowson, Jerry	OW	FTS-382-7818	(202)-382
Cannell, John	OWEP	FTS-475-9539	(202)-475
Conlon, Mike	OWRS	FTS-382-5400	(202)-382
Frederick, Rod	OWRS	FTS-382-7051	(202)-382
Grubbs, Geoff	OWRS	FTS-382-7040	(202)-382
Newton, Bruce	OWRS	FTS-382-7060	(202)-382
Southerland, Betsy	OWRS	FTS-382-7046	(202)-382
Taylor, Phill	OWRS	FTS-382-7046	(202)-382
Warner, Cindy	OWRS	FTS-382-7051	(202)-382
Higgins, John	Reg. II	FTS-340-6680	(201)-321
Siegal, Abe	Reg. II	FTS-264-4753	(212)-264
Voyce, Lisa	Reg. II	FTS-264-4124	(212)-264
Kanetsky, Charles	Reg. III	FTS-597-8176	(215)-597
Nelson Zandi, Ava	Reg. III	FTS-597-9388	(215)-597
Collins, George	Reg. IV	FTS-257-3402	(404)-347
Leedy, Forrest	Reg. IV	FTS-257-3012	(404)-347
Anagnost, John	Reg. V	FTS-886-0143	(312)-886
Goranson, Steve	Reg. V	FTS-353-2074	(212)-353
Melville, Bill	Reg. V	FTS-886-1504	(312)-886
Holman, Mac	Reg. VI	FTS-255-2289	(214)-655
Holloway, Tom	Reg. VII	FTS-757-3884	(913)-236
Wilson, Eric	Reg. IX	FTS-454-8312	(415)-974

FTS - Federal Telephone System

systems. Future success in these areas will depend on the ability to maintain communication with system managers, program managers, and priority data system users.

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ANALYSIS AND INTEGRATION OF ECOLOGICAL MONITORING DATA

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ABSTRACT

The US Environmental Protection Agency Environmental Monitoring and Assessment Program (EMAP) is designed to sample ecological regions and processes and to prepare evaluations of the trends and ecological health of these regions and the nation as a whole. In the process of being implemented, EMAP is divided into seven ecoregion and media Technical Groups (TGs). Each of these TGs will collect and analyze ecological data. Analysis of the data will be carried out using both statistical and spatial analysis tools. Another element of the program integrate the TG results across ecoregions on larger spatial scales.

An innovative data management concept has been devised to facilitate the efficient identification, collection, aggregation, and analysis of data in this physically distributed environment. A single logical data base composed of multiple, geographically distributed physical data bases is used for data storage and manipulation. A centralized Data Set Index (DSI) is utilized to manage the logical data base and to coordinate the data management activities in the TGs.

The DSI structure is a part of the EMAP Information System which includes additional modules for data handling, data analysis, communications, publications, and program management. The EMAP Information System creates a single management entity to control and direct the data management actions of all units in the program through a variety of techniques.

Advanced technical analysis capabilities such as Geographic Information Systems (GIS), remote sensing capabilities, statistical packages and some recently developed PC-based systems are included to facilitate the understanding and analysis of the data.

INTRODUCTION

The US Environmental Protection Agency Environmental Monitoring and Assessment Program (EMAP) is designed to sample ecological regions and processes and to prepare evaluations of the trends and ecological health of these regions and the nation as a whole.[1] In the process of being implemented, EMAP is divided into seven ecoregion and media Technical Groups (TGs). The seven ecoregion and media groups (forests, wetlands, lakes and streams, agroecosystems, and near coastal ecosystems and air and deposition and groundwater media) will collect data from existing sources and augment them as necessary for regional assessments of the status and trends of ecological resources and pollutant exposures. These assessments will be aggregated and collated by the Integration Group to form an index of ecological health across ecoregions and media groups. The seven TGs (and the Integration team) are physically distributed across the country in various laboratories.

The normal difficulties encountered in the design and implementation of a data management system to store and manipulate monitoring data are complicated by three additional factors in EMAP: 1)the user community is geographically distributed across the county, 2)the outputs and uses of the data are not defined, and 3)new analysis techniques will be necessary in the understanding of data. Each of the TGs has a distributed structure that includes other laboratories and various university faculty members as consultants. The types of data to be collected have been partially identified and some have been collected. The forms of analysis and the outputs of the analysis have not been identified and indications are that the analysis process will be continually altered through the life of the project. GIS is an emerging technology and few standardized techniques have been developed.

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The scientific user community is generally familiar with computers and data bases. The advanced technologies that are necessary for the analysis process are generally 'user-unfriendly' and do not lend themselves to routine repetetive processing modes. The large quantities of data to be processed and the complexities of some of the analysis systems do not always lend themselves toward PC-based hardware. Minicomputer systems will be necessary to manipulate and share the data sets in the system.

There are problems in keeping large centralized data management systems responsive to user needs. Although a number of techniques are available to overcome these difficulties,[2] the constraints imposed by a research environment with a constantly evolving use of data, effectively eliminated these approaches. A data management system must deliver ecological data to the researchers in an efficient, effective manner.[3]

DATA MANAGEMENT ORGANIZATION

A new structure has been devised to implement data management activities for this distributed environment headed by a central Data Management Coordinator (DMC) reporting to the Program Manager. A new Data Analyst function was invented and located in each of the Task Groups reporting to the DMC. An additional Data Analyst function supports the Integration Team. These data analysts are, in turn, supported by a variety of technical experts in the various analytical methodologies employed.

The DMC's principle function is to provide overall direction and coordination for the data analysts and the technical experts. The DMC serves as a source of data management information for the EMAP Program Manager. The DMC identifies the technical experts and establishes the lines of communication between the technical experts and the data analysts.

To facilitate this coordination and communication of information the DMC serves as team leader for the Data Management Coordination Group (DMCG). The DMCG is composed of the DMC, the Data Analysts and the technical experts.

The Data Analysts are located in the TGs. They have expertise in the work of the eclogical science research group and are also skilled in data management technologies. Data management functions within each TG are thereby tailored to the work being performed by the TG members. Although individual TGs approach data management tasks quite differently, several common functions exist for all data analysts. They are all responsible for the creation of TG specific data bases, for operation and maintenance of TG data bases, for movement of data into and out of TG data bases, and for assisting TG members with data analysis and the identification of useable data bases.

In addition to the responsibilities the data analyst has with respect to the TG, the data analyst is also responsible to the DMC. As a member of the DMCG the data analyst's responsibilities include; the recording of all data base acquisitions, movements, usage, and other information into the DSI, the communication to the DMCG of all information that may be of use to members of the other TGs, following the standard practices defined by the DMC to assist data integration efforts, and assisting with the integration of the TG data with data from other TGs.

Technical experts provide the skills necessary to utilize advanced analysis techniques. It was discovered that it was unrealistic to expect all data analysts, who are experts in the technical fields of their TG to also have expertise in all of the myriad data analysis packages available. The technical experts are identified at each operating location and act in the role of consultants to the data analysts.

EMAP INFORMATION SYSTEM CONCEPTUAL DESIGN

The goal of the data base design for EMAP was to incorporate a diverse data universe into a system that made the data appear as a single entity. The EMAP Information System has been designed using a conventional top-down structured analysis approach dividing the tasks into modules based on function. Initially the overall needs of the EMAP project personnel (scientists and management) were identified and categorized by function. This defined the scope and

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provided a superstructure from which all further functional modules could be built. The structure consists of the following 6 categories: 1) the Data Set Index, 2) data handling, 3) data analysis, 4) communications, 5) document composition, and 6) program management. Note that only the second and third categories deal with environmental monitoring data per se. The others all deal with information about the data and projects (metadata) that is required to integrate the distributed personnel and data resources of EMAP into a single logical data management system.

While the EMAP Information System design proceeded from a top down approach the data base design section was approached from the bottom up. This bottom up data base design was utilized because most of the monitoring data systems for EMAP already exist and their structures must be taken into account in the design phase.

A bottom-up approach also insured that the data requirements and processes of the users determined the design of the data base. This insured the responsiveness of the system to user needs. A design that includes the user requirements as the paramount parameter is almost always more responsive to the users needs. A series of interviews with the user community helped to establish the approaches and methodologies of the user community. The commonalities through this process became the foundation for the design of the data base.

The EMAP Information System is depicted in Figure 1, with each of the principal functions of the design represented as a separate block.

Data Set Index (DSI) Module

The DSI can be viewed as the EMAP data base. It is a data base containing information about EMAP data. It is the mechanism that ties the multiple, geographically distributed physical data bases together into a single logical data base. The DSI identifies the uses and location of all data sets in EMAP. It contains information about the data sets spatial and temporal extent, parameters, usefulness, and quality. The DSI tracks and identifies the sources of data and monitors

the movement of data throughout the EMAP information system.

Data sets are classified by the level of use by EMAP projects. The four levels of EMAP usage are: investigated, accessed, acquired, and generated (Figure 2). At the "investigated" level the data set has been investigated for use by EMAP personnel but is not being used or referenced in EMAP projects. At the "accessed" level some of the data from the data set has been used or referenced by EMAP projects but the data is not stored permanently in the EMAP information system. At the "acquired" level some or all of the data from the data set has been acquired for EMAP use and is being stored in the EMAP information system. At the "generated" level the data set has been designed and populated with EMAP data and is stored in the EMAP information system.

The information about data sets entered into the DSI is divided into 5 categories:

1. Information about the data set such as the name of the data name of the data set, a description of the data set, the source of the data set, and the data set parameters.

2. Information to assist in data retrieval such as acronyms for the data set name and parameters, keywords used to reference the data set, and spatial and temporal extent of the data set.

3. Information about the person or group making the DSI entry such as their name, level of understanding of the data set, and their task group affiliation.

4. Information about the uses and/or usefulness of data to EMAP such as the potential usefulness of investigated data, uses of the acquired data, and the name of the person or group using the data.

5. Information about the acquisition and storage of the acquired or generated data such as the location of the data, name of the data analyst in charge of the data, and the formats in which the data is stored.

The DSI requires different information for each level of EMAP data set usage. At the "investigated" level the information required

Figure 1. Overview of the EMAP Information System

Universe of Data Sets

Data sets outside of EMAP domain. Not yet investigated for use by EMAP personnel.

EMAP Investigated Level

Existing data sets investigated by EMAP personnel but not yet used or referenced in EMAP projects.

EMAP Accessed Level

Data sets accessed, used, and/or referenced by EMAP personnel but not stored permanently in the EMAP information system.

EMAP Acquired and Generated Levels

Data sets acquired by EMAP and maintained permanently in the EMAP information system.

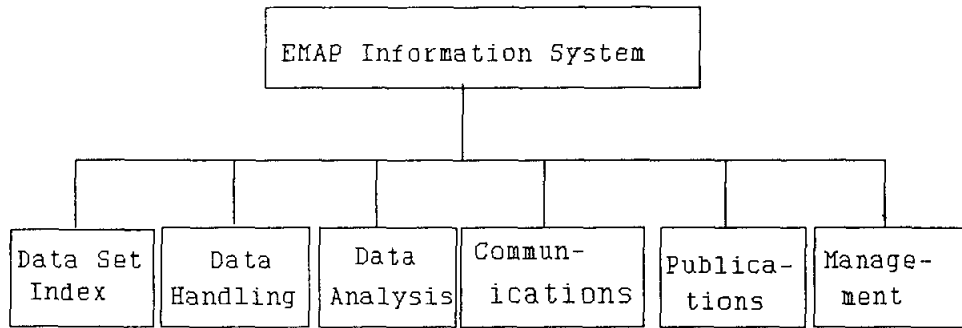EMAP generated data sets designed and populated with EMAP data and stored in the EMAP information system.

Figure 2. Description of and Relationships between Levels of EMAP Data Usage.

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falls into categories 1,2, and 3 and with only the minimum amount of detail. As the level of EMAP usage increases to "acquired" and "generated" the information from all 5 categories is required and the amount of detail within each category increases (Figure 3).

The DSI describes and tracks data set movement, data set formats, and includes an index of the level of understanding possessed by the person making the DSI entry. The DSI contains information about the movement of data within the EMAP system. Data analysts are required to enter into the DSI any information relating to the transfer of data within the EMAP system or out of the EMAP system. This information serves as an audit trail for data sets once they have entered the EMAP system.

Every descriptive entry made in the DSI is affected by the level of understanding of the data the individual making the entry. An index of understanding is included with every descriptive entry into the DSI. This indication of the depth of understanding of the data gives a later user a quantifiable degree of confidence in the description. This degree of understanding index is a numeric grade from 1 (low) to 5 (high).

Index
Value   Level of Understanding

1   Entry is based on knowledge of only the name and identification of the data base.

2   Source of the data has been contacted and has provided input to verify the description of the data.

3   The data have been reviewed to determine the ranges and types of characteristics encountered.

4   The data have been reviewed and written description of the data has been extracted from an abstract provided by the originator of the data.

5   Entry is based on a thorough knowledge of the contents of the data base, including history, ranges of values, temporal and spatial characteristics, etc.

The DSI is searchable by key word or combinations of key words. As the index grows, however, retrievals based on a key word approach will become less successful due to different spellings of words, abbreviations, or miscoding. A hyper-text facility is utilized to cross-reference the parameters, temporal, and spatial descriptions of the data. Hyper-text allows the data base to locate the logical siblings of each entry. This allows the user to locate and identify all other data sets that share one or more of these characteristics. Part of the hyper-text facility is a table to cross-reference different methods of describing the same thing. This cross-reference list is maintained by the central DMC.

The DSI stores information on the formats of data sets as they enter the EMAP Information System. In addition, the DSI contains information about the existence and location of software used to reformat data sets. This information is accessible to all users allowing them to see if software exists to reformat a data set to a format they may need for import to EMAP or export to some external analysis package.

The Quality Assurance of each data set in the DSI is described in at least two ways: the QA component of the individual data points is described and the QA of the data set taken as a whole is also described. We have discovered that many monitoring data sets are created through collection and analysis procedures that are well documented and performed in a standard manner. The data set could be said to have a high QA component. Taken as a whole, the data characterize the site rather thoroughly. At the same time, there may be certain statistical outliers (both above and below) that, if taken individually, could give an erroneous picture of the site. Therefore, individual values may be more suspect than the picture given by the data set as a whole.

Data Handling Module

The primary functions of this module are data transfer, data formatting, and data editing. Integrated with the data editing function is a user definable data consistency checking capability. There are three major functions associated with data transfer in any system; importing, exporting, and moving data around inside the system. All transfers of

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┌─── Universe of Data Sets ──────────────────────┐  Amount
│                                                 │     of
│        No DSI information required.             │  detail
│                                                 │    per
│   ┌─── EMAP Investigated Level ─────────────┐   │   info
│   │                                         │   │ category
│   │      Data set information.              │   │
│   │      Retrieval assistance information.  │   │   │low
│   │      Data entry person information.     │   │   │
│   │                                         │   │   │
│   │   ┌── EMAP Accessed Level ──────────┐   │   │   │
│   │   │                                 │   │   │   │
│   │   │   Data set information.         │   │   │   │
│   │   │   Retrieval assistance information.│  │   │   │
│   │   │   Data entry person information.│   │   │   │
│   │   │   EMAP uses/usefulness information.│ │   │   │
│   │   │                                 │   │   │   │
│   │   │ ┌── EMAP Acquired and Generated Levels ─┐│   │
│   │   │ │                               │ │   │   │
│   │   │ │ Data set information.         │ │   │   │
│   │   │ │ Retrieval assistance information.│ │   │
│   │   │ │ Data entry person information.│ │   │   │
│   │   │ │ EMAP uses/usefulness information.│ │   │
│   │   │ │ EMAP acquisition and storage info.│ │   │high
│   │   │ └───────────────────────────────┘ │   │   ↓
│   │   └─────────────────────────────────┘   │   │
│   └─────────────────────────────────────────┘   │
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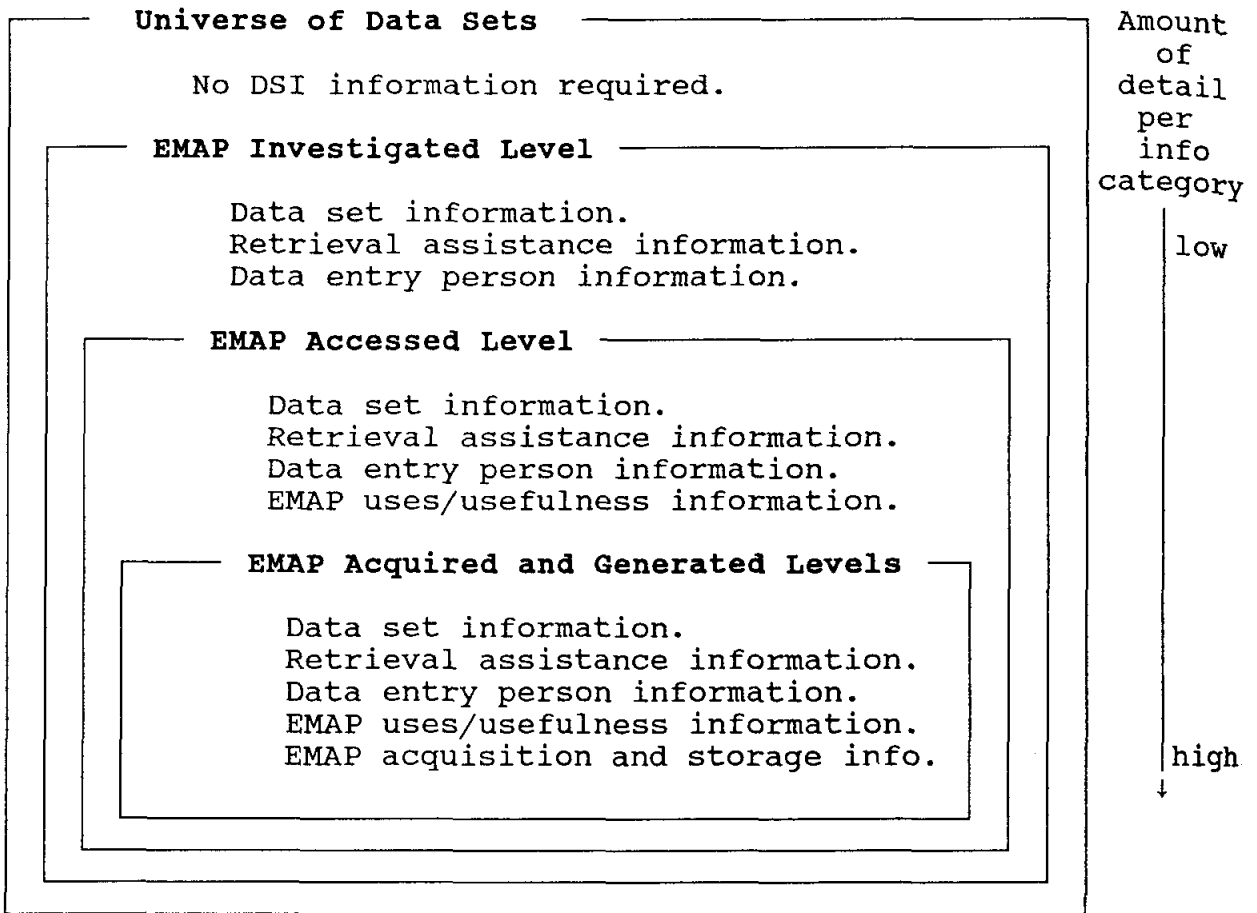
Figure 3. Relationship between Levels of EMAP Data Usage and DSI Information Requirements.

data are recorded in the DSI. Data compression techniques are used to reduce the volume and time required for data transfer through the system. For large data sets, or data sets isolated from network access, data transfer may be by magnetic or, as technology develops, optical medium.

Data sets are imported directly into the data base of the TG using them. The importation of spatial data from non-digital sources by scanning devices must meet GIS standards. Non-digitized data are imported through a module for user designable screens. This allows users to design input screens that are easy to understand for their data entry clerks and may be customized for any particular application. User definable data range checks may be added to check the reasonableness of the entered data.

The transfer of data within the system is normally through the EPA network. A compression routine is used to compress data for transfer when it is desireable to reduce network traffic and transfer times. The PKPAK and NARC routines available through shareware are distributed by the DMC to each operating location.

To retain data integrity, only one official copy of a data set is in the system at a time. Temporary working copies may be made from time to time but only the immediate users will be aware of their presence. Any change made to a data set either updates the official version or creates a new data set. These activities are tracked through the DSI.

When an ASCII record format is not available for data transfer the data analyst and the DMC develop methods for importing the data and adds the developed method to the data import/export library. Information about the original format of the data prior to its entry into the EMAP information system is recorded in the DSI.

The movement of data to systems outside EMAP is a necessary step in supplying data to many of the user specific analytical tools such as models. The system normally exports data in an ASCII format by default. Additional export formats may be added to the system's import/export library as required. For spatial information the default export format is the ARC/INFO export format.[4]

A user definable import/export module allows users to define the record formats of data needing to be imported/exported. This is useful in formatting export data for other applications and for bringing data sets into the system that have formats other than those recognized by the system. The user has the ability to save these formats for future use or have the data analyst add them to the system's import/export library.

The system allows users to supply algorithms for testing the reasonableness of data and provides simple checks such as range and difference checks. The data editing process is integrated with the consistency and validity checking components to allow immediate modification of values flagged as unreasonable. User supplied algorithms that have broad application are submitted for inclusion in the EMAP system.

The editor is fully integrated with a graphing and mapping module. The actual editing of the data takes place in a text mode but the graphics tools are available to help the user identify problems with the data. The user has access to data manipulation tools that will allow the user to perform algebraic functions between parameters and save the results as a new parameter.

The editor allows viewing of some data by plot and table simultaneously. Any data point being viewed is editable via the table window with changes to the data immediately reflected in both the table and the plot windows. Data flagged as unreasonable by the consistency checks are clearly indicated in both the table and the plot windows. The user is able to select more than one parameter at a time to be viewed and edited. The ability to view several parameters simultaneously to assist the user in checking the data for reasonableness.

As another tool to check the reasonableness of the data the editor has the ability to overlay the data on a base map to help identify incorrect spatial information and help to identify unreasonable spatial trends. The data that is found to be unreasonable can be identified and corrected without leaving the editing module. More than one parameter containing spatial information can be viewed and edited simultaneously. The user is able to view tables of data for any location for any parameter and edit the table.

The changes made to the table are immediately be reflected in the spatial reference window for that parameter at that location.

Data Analysis Module

The data analysis module consists of four major functional areas: statistical analysis, spatial analysis, contouring, and graphing and charting. In addition to these analytical tools the system allows users to define custom algorithms for data analysis. User algorithms with wide application may be submitted through the data analysts for inclusion in the system. The user has the option of running all analyses in an interactive or batch mode. Analysis of data is normally customized by the user to his own requirements. Some sources to conventional software packages is provided in EMAP.

Routine statistical analysis is performed by commercially available software, principally SAS[5]. This system provides all of the normal statistical parameters and has its own data management system. Links to SAS are relatively transparent to the user and if data must be reformatted prior to statistical processing the system performs the task.

The spatial analysis module provides a range of spatial analysis tools from quick data overlay on base maps for site location to publication quality maps representing detailed data analysis in a spatial framework. The module consists of 3 main categories of spatial analysis tools: a raster based GIS, a vector based GIS, and a user-friendly mapping system. Any new data coverages resulting from spatial analysis are treated as a new data set and the user may store it in the system.

The ERDAS[6] raster based GIS software provides users with the ability to analyze spatial data that is in raster format such as landsat data and other remotely sensed data. In addition, ERDAS is capable of converting the raster based GIS data to vector format that can be used in the EMAP information system's vector based GIS.

The principle vector based GIS used is ARC/INFO software[7]. It is used for complex spatial analysis, production of high quality

map outputs, and efficient storage of spatial information. ARC/INFO is capable of accepting vectorized data from the raster based GIS and will produce rasterized data from vector data for movement to the raster GIS.

A user-friendly module utilizes GeoVision, Inc.[8] software, an easy to use PC-based system for simple data overlay on base maps to produce location maps or to perform simple spatial analyses. It is a 1:2,000,000 map of the US on a CD-ROM along with software to locate places, create overlays, identify coordinates, etc. It is used to produce maps for scientific analysis and draft reports. Outputs from this system may be fed directly into ARC-INFO for transfer to others and for high quality outputs.

Three contouring systems are integrated with the mapping and GIS systems to allow production of both 2 and 3 dimensional contour maps with the overlays of base map information. The contouring module provides a link to Dynamic Graphics Interactive Surface Modeling (ISM)[9], ARC/INFO TIN, and EPA's GEO-EAS[10] contouring systems. The system allows users to store the contoured data as a coverage data set updating the DSI. The contoured data is geo-referenced when stored to allow for future use in GIS analysis.

The graphing and charting module provides users with tools for producing bar charts, pie charts, line graphs, X-Y plots, and other methods of graphically representing data. The module is easy to use and requires a minimal amount of user training. The module is composed of various commercially available graphing and charting packages such as SAS-GRAPH[11], Lotus Graphwriter II[12], and Voyager[13]. Graphics produced by the system are available for output on various devices or to disk files for storage and later retrieval. The output file formats are compatible with the system's graphics editors and desktop publishing modules.

The tabling module provides users with several tabling formats to display the data as well as allow users to design their own tables. Table formats designed by the user that have common use can be submitted to the data analyst for addition to the system.

Communications module

Central to the management of any large distributed information system is a standard method of communication between all the personnel involved with the management task. Although telephone conversations are convenient, they are often ineffective because they may lack the level of information and recording requirements necessary for a management task of this size and complexity. The standard method of communication for the management of the system is via electronic mail (EMAIL) and all important information is communicated using this method.

EMAP utilizes EPAs EMAIL system as a backbone for communications, however it is tailored by the addition of customized distribution lists. All participants in EMAP have their own EMAIL address. Each TG established custom distribution lists for its members. A bulletin board is established to communicate general information about the EMAP program to interested personnel both inside and outside of the EMAP project. This bulletin board is open to all requesting parties for reading and is managed through the central EMAP contact.

Publications Module

This module provides basic style formats for reports and presentation materials and also allows users to design their own style formats. Style formats for common journal outlets are added to the system with the coordination of the data analyst.

A desktop publishing sub-system is used to produce documents for rough draft as and final publication. It consists of a word processing component and a page composition component. The word processing component is Word Perfect 5.0[14] which provides a spell checker and on-line thesaurus in addition to advanced word processing functions such as automatic production of indices, table of contents, and pagination. The page composition component aids the scientist with the design and layout of a document. It is capable of integrating graphics files produced in EMAP with text produced in the word processing system. It includes a graphics editor, the ability to receive scanned input for incorporating printed graphics, and a drawing

subsystem to allow freehand drawings. The freehand drawing feature allows rough sketches of graphics to be entered into a document for review purposes. These rough sketches will allow reviewers to get a feel for the final document, design and layout, without having to wait for the final graphics to be produced. Later the final graphics can replace the rough freehand sketches.

A routing module's function is to record information about the development of documents from first draft to publication, basically an audit trail of the review process. This assists scientists and managers in monitoring the progress of reports. It also allows management to identify bottlenecks in the review process and to develop a clearer picture of the status of reports for the entire EMAP project. The system is able to generate summary reports on the number of papers proposed, in first draft, in pier review, and awaiting publication. The reports are able to be output by subcategories such as by author, subject, reviewer or publication outlet.

The DMC has made Referee[15] software available to the various originators of documents in EMAP. This PC-based system provides a bibliographic capability for documents and is capable of creating cross-reference lists of documents used.

After a report is published it is removed from the routing system and an entry is made in the EMAP bibliography system. This system is maintained by the DMC and serves as a reference for all EMAP personnel to locate project publications. It provides management with an overview of the types of publications, the subject areas, and the researchers involved with the publishing process in EMAP.

An easy to use slide and overhead production system for making presentation quality materials is also available to the users. The system incorporates any graphic produced by other modules of the EMAP information system. It is capable of producing high quality word charts in a wide variety of formats.

Management module

The management system provides a means for managing information on personnel,

budgeting, and project scheduling, and provides concise output for review and analysis.

The Contact Tracking System module is used to record who contacted whom about what subject and when and how the contact took place. Its principal function is to track and document who has been briefed on the mission of EMAP. The centralized data base is implemented on the EMAIL system. It is the responsibility of EMAP personnel to update the data base when other modes of communication take place (i.e. telephone, meetings, U.S. Mail, etc.). Used correctly, this module assists both scientists and management in checking to see that appropriate contacts have been made about various subjects.

The personnel module stores all information on EMAP personnel such as name, phone number, organization, contract, funding sources, project responsibilities, title, supervisor, committee membership, and other details. Retrievals are available by any element and output in a predefined or user definable table format.

The budgeting module provides management with a tool for monitoring the availability of funds with relation to the projects obligated funds and expenditures. The system is easy to use while being capable of accommodating the most detailed of budgeting requirements.

The project scheduler module is used by management to develop project timelines and milestones so managers can monitor the progress of each EMAP project. This system will be integrated with the budgeting module to allow managers to visualize how projects are progressing relative to the their budgets.

CONCLUSIONS

It is evident that data management of ecological data in a geographically distributed environment requires non-standard solutions. We have found that a centralized repository of data is not responsive to user needs. Although technically feasible, this approach requires an unrealistic degree of coordination between sites.

Data management for scientific research, is, by its very nature, not able to predefine uses of data or outputs. The operation of understanding what data represent is complex and requires a capability to manipulate and view data in multiple formats and from multiple viewpoints. This capability requires a real-time ability to manipulate and edit data to create multiple views of the data in the time-space-parameter environment.

Decentralized data bases and data management require centralized coordination to eliminate duplications of effort and to manage the flow of data into and out of the system. Program management relies on a single source for data management activities. A data set index has proved successful in this.

Commercial software that provides analysis of complex ecological data in a responsive manner is presently evolving. A priority function of data management is keeping up with this rapid evolution and passing these technologies to the users.

Quality assurance of data must be thoroughly documented and must include references to the quality of the data points in the data base as well as to the overall quality of a database.

DISCLAIMER

Mention of trade names or commercial products does not constitute endorsement of recommendation for use by either NSI Technology Services Corporation or the United States Environment Protection Agency.

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Managing Data/
Reporting Information

DATA MANAGEMENT FOR A FEDERAL SUPERFUND SITE:
A Practical Perspective

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ABSTRACT

A plan for management of environmental groundwater quality information was prepared as part of a remedial investigation (RI) for a federal Superfund site located in California's San Joaquin Valley. A process of establishing data quality objectives was developed and used to optimize the level of quality control to be provided by the data management system in coordination with an independent analytical laboratory. A computer-aided system was developed for sequentially 1) checking an American Standard Code for Information Interchange (ASCII) or other word prosessing text file analytical report-form data package from the laboratory for completeness, 2) reformatting the data and performing quality control checks on the data package using Lotus 1-2-3[1] software, and 3) translating selected records from Lotus 1-2-3 and appending these records to a relational database maintained using dBase III Plus[2] software.

The relational database is used to produce reports of uniform data quality for further analysis, as ASCII or other word processing text files for inclusion into documents, and to satisfy routine inquiries. The data management system minimizes the potential for transcription errors or other non-systematic data quality degradation. Anticipated improvements to the existing system include dissemination of the database on a subscription basis to other users. The San Joaquin Valley site data management program serves as a prototype for similar water quality information systems.

INTRODUCTION

Groundwater quality monitoring for a federal Superfund site can result in a significant volume of information. Monitoring for one such site in California's San Joaquin Valley occurs quarterly, includes collection of water samples from as many as 70 wells, and generates laboratory results from performance of as many as five different U.S. Environmental Protection Agency (EPA) analytical methods per sample, each of which is capable of detecting as many as 20 different chemical compounds. Each sampling round also includes laboratory analysis of necessary quality assurance and quality control (QA/QC) samples such that the quarterly data volume can approach 500 pages of laboratory report sheets.

Because the laboratory analytical data are printed using a computer, and subsequently interpreted and presented using computers, the potential for digital information transfer is apparent. The data quality objectives established for the project, which require a high standard of quality assurance in interpretation and presentation, make digital information transfer an economic necessity.

DATA QUALITY OBJECTIVES

Fundamentally, data quality objectives (DQOs) (EPA 1987) define an economic incentive for management of water quality information. If the expected cost of possible errors exceeds that of a more reliable information management program, the new

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program is economically justified. DQOs are established for both the analytical laboratory and for the technical database established for the site.

LABORATORY DQOs

One laboratory is used for the majority of groundwater quality analyses performed on a San Joaquin Valley Superfund project managed by Kennedy/Jenks/Chilton. Laboratory DQOs are implicitly established by the EPA in design and publication of the analytical procedures used (EPA 1979, EPA 1983). These include the objectives of complete identification and quantification of detectable concentrations of chemicals in a pre-defined list for each specific analytical method (EPA 1984).

Additional laboratory DQOs are established for other quality assurance purposes. These DQOs result in the analysis of laboratory blanks, laboratory spiked samples, and laboratory replicate samples (EPA 1979). These DQOs include numerical criteria for the assurance of repeatability, accuracy, precision, and representativeness in analysis of environmental samples (Keith 1988). These objectives are similar for most of the laboratories involved in hazardous substance sample analysis (Einerson and Pei 1988).

In addition, the laboratories perform a number of daily quality assurance analyses in compliance with California Department of Health Services (DHS) protocols under the hazardous waste laboratory certification program. These include daily performance of standarization and calibration procedures and detailed control chart record-keeping.

Certain project-specific laboratory DQOs are also established. For the San Joaquin Valley Superfund site, these include the requirement that detection limits for all compounds remain at or below applicable water quality criteria. For example, although chloroform may be detected in a given sample at a concentration of 50 micrograms per liter (μg/L, parts per billion), a concentration in below the acceptable drinking water level (ADWL) of 100 μg/L established for that

chemical for that site by the DHS, the laboratory may have to assure that a much lesser concentration of dibromochloropropane (DBCP) could be detected as well, if present at a concentration of more than 0.2 ug/L. This is true because the intent of monitoring some of the wells near the San Joaquin Valley site is not the identification and quantification of volatile organic compounds (VOCs) in water samples; rather, it is the identification of households whose well-water quality warrants the provision of an alternate supply.

Finally, the sheer volume of information involved necessitates that certain logistical objectives be achieved. A data package, typically consisting of hard-copy and floppy disks containing ASCII or word processing text files of laboratory analysis reports (for all environmental and QA/QC samples and for all analyses requested during a given sampling round) must be complete and internally consistent before it is accepted from the laboratory. In some instances, subsets of the complete data package are requested for priority delivery, but they are explicitly defined as such on the analysis request forms and must satisfy the same completeness and consistency criteria before they are accepted from the laboratory for inclusion into the database.

For the San Jaoquin Valley site the laboratory analysis report forms are managed by computer. Therefore, an agreement was reached at the inception of the project regarding the format and organization of data files and the reports themselves. These specifications are documented in the quality assurance project plan prepared for the site.

DATABASE DQOs

The primary DQO of the database is preservation of the quality of information as delivered by the laboratory. The greatest level of quality at which the information can be conveyed in that which is provided in the certified laboratory analytical report (Ward et al. 1988). The efforts described below were developed with the intent to preserve the quality of collected information by avoiding the database quality degradation that

transcription errors, omissions and other possible non-systematic errors could yield without such a system.

COMPUTER-BASED DATA MANAGEMENT SYSTEM

Given a complete and consistent data package from the laboratory, data management is implemented by extracting information from the ASCII or word processing text files used to print the certified laboratory analysis reports, rearranging the data into the record format of an existing database, and appending these new records to a working version of the site historical water quality database. These steps are typically accomplished using a number of publicly-available software packages and IBM AT^3-compatible computers.

The laboratory used for the San Joaquin Valley site produces analytical reports in a consistent format using an IBM PC^4-compatible word processing package which stores files in ASCII format. These files are arranged such that each analysis performed on a given sample in a given sampling round is reported in one file. Therefore, each sample can be tracked by a filename in the raw data package. Initially, the entire raw data package is duplicated onto working floppy disks. The original disks received from the laboratory are placed in an envelope and placed in the job file along with the original hard copy report sheets received in the data package. The number of disk files is then compared with the number of sample analyses requested, laboratory QA/QC samples anticipated, and the number of hard copy reports received. Assuming that the data package is complete, the floppy disk files are then opened using an ASCII based work processing package (Wordstar^5) and certain common character sequences are globally replaced. For example, a standard representation of a non-detectable results for a given chemical in the San Joaquin Valley Superfund laboratory's report is:

Detection Limit
Result   (ug/L)

ND   0.2

In order to preserve the information provided, namely that a specific chemical was not present above a specific concentration, the non-detect is combined with the detection limit and converted to a numeric format from the character format (ND) for inclusion into the numeric field in the database. This non-detectable result then appears as shown below:

Detection Limit
Result   (ug/L)

-0.2

Needless to say, the only results which appear in the database with negative values are non-detects. The global replacement of character formats with numeric formats for non-detectable results is performed by Superkey^6 macro program such that it can be done sequentially on a large number of files and that no inadvertent additions to or subtractions from the raw data files are made. Other laboratories report data in different formats, each of which is addressed on a project-by-project basis.

A key portion of the planning which goes into establishing DQOs and quality assurance project planning for a given project is the agreement regarding laboratory report formats which are modified as needed and in order that they remain consistent through the duration of the project.

The numerically configured San Joaquin Valley site data files are imported as text into a template Lotus 1-2-3 worksheet which contains a number of data management macro routines. This file transfer is handled by the Superkey master program. The 1-2-3 routines parse the imported text into character and numeric information in separate columns, perform data query operations to compensate for the different analytical methods employed on each sample, and copy extracted data to a specified, named portion of the worksheet for later translation as records into the file-format of the database. Each processed data file is saved as a 1-2-3 worksheet file.

The master macro program sequentially operates on each raw data file until all have

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been saved as worksheets. The program then transfers control to the Lotus translate utility. Only release 2.01 of Lotus 1-2-3 has the translate capability to handle the large record length of this project database.

The translate utility program sequentially translates the named specified range of each data worksheet file for Lotus 1-2-3 release 2.01 format to that of dBase III Plus. Once this translation occurs, the master macro exits Lotus, enters dBase III Plus, and using the working version of the current database, appends each one-record file from the sequence of files created for that sampling round. A working version of the current database is used in order to check the database for an accurate data transfer of new information prior to archiving it as the new project database.

The databases for other projects are augmented similarly. The particular characteristics of the analyses performed, the frequency of sampling, and the laboratory report formats used for a given project are used to determine the optimum logistics of digital data management.

DATABASE STRUCTURE

The San Joaquin Valley site groundwater quality database is structured to include the unique sample identification code assigned to each sample upon collection, the identification number for the well from which the sample was collected, the date sampled, the quarter and year of the sampling round, the sampling entity, the analyzing laboratory, the laboratory's sample identification number, and the analytical results for the sample.

At the inception of the project, the database was structured to accept only those chemicals previously detected in water samples from the site and vicinity. Two problems with this approach were identified which justified the creation of a more holistic database structure. The first problem identified was that with the passage of time, new chemicals were occasionally detected and the database had to be restructured with each new detection. The second problem was that the value of a fully descriptive database,

wherein non-detectable values (and implicitly detection limits) were as easily sorted and reported as were detectable values, became apparent. For example, historic analyses of groundwater samples from the San Joaquin Valley site for the compound Dinoseb (dinitrobutylphenol, DNBP) were historically, as they are now, performed using gas chromatography (GC) by EPA Method 615. However, analytical reports only listed the result for Dinoseb. The question of whether other compounds detectable by EPA Method 615 were detected in the analyses performed required an audit of historical raw instrument analytical data (chromatograms). Therefore, the current version of the database, and the prototype for other project databases, is structured to include results for all chemicals commonly detectable by the analytical methods employed. As the list of analytical methods to which samples are subjected grows, the database is restructured. This can result in very large databases, sparsely poulated by detected values, but a large volume of non-detectable results can be a significant asset in a Superfund site investigation.

USES OF DATABASES

Project water quality databases are used for a variety of purposes. At a minimum, such databases are used to speed the production and presentation of monitoring reports which must be submitted to involved regulatory agencies. By using a database of assured quality as the source of information to be presented in tables and on figures, the monitoring reports are internally consistent and easier to prepare.

The same attributes which make routine reporting more efficient when using a project database also make further data analysis and interpretation easier given the availability of computer-based tools for such analysis. ASCII-file reports can quickly and easily be produced from the database and imported into worksheets, graphics packages, or numerical model input files with little risk of transcription errors. The possible errors which can occur in such large-scale data-block transfer operations are systematic errors which are much more easily detected than are

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irregular non-systematic errors like a transposed number or a typographic error.

POTENTIAL IMPROVEMENTS

Potential improvements to the San Joaquin Valley site groundwater quality database and data management system have, to some extent, been implemented on other project databases which used the first as a prototype. These include more extensive changes in the laboratory report forms to better facilitate information-handling in the template worksheet, and changes to worksheet structure to allow automated calculation of sample holding times between collection, extraction, and analysis of the extract in the laboratory. Additional imporvements anticipated include a document/disk control system to allow floppy-disks containing the current database to be distributed to parties needing access to such information on a periodic basis, or dial-up access to a current database for the same purpose.

The data management process is also applicable to information derived from soil sampling and laboratory analysis. As the opportunity arises, a comprehensive database which integrates chemical analytical results with the spatial and lithologic relationships implicit in a soil characterization investigation will be established. A key to implementation of such a database is the availability of IBM PC-compatible graphical presentation software which can preserve spatial location information while illustrating chemical concentration data. Such software is common for geologic exploration, but is not often implemented on PCs and is not frequently coupled with such a large potential volume of data from chemical analysis.

CONCLUSIONS

A comprehensive data management program for assuring the reliable storage and dissemination of a large volume of existing and anticipated groundwater quality information was established on the basis of apparent feasibility and economic incentives. The data management program utilizes the

benefits of quality assurance project planning to establish data quality objectives (DQOs), communication protocols between the analytical laboratory and the database manager, and a documented protocol for data package configuration and transfer. The data management program is successful for the project under which it was first implemented, and has successfully served as a prototype for other project water quality databases.

The exisiting data management system will be enhanced to include additional automation in QA/QC calculations, and the ability to provide magnetic media containing the current database to project data users on a subscription basis. Future data management systems are planned which will integrate three dimensional spatial and lithologic information with similar multi-dimensional chemical databases for soil characterization projects.

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ENDNOTES

[1]Lotus 1-2-3 is a registered trademark of the Lotus Development Corporation.

[2]dBase is a registered trademark and dBase III Plus is a trademark of the Ashton-Tate Corporation.

[3]IBM AT is a product of the International Business Machines Corporation.

[4]IBM PC is a product of the International Business Machines Corporation.

[5]Wordstar is a registered trademark of the MicroPro International Corporation.

[6]Superkey is a registered trademark of the Borland International Corporation.

DATA MANAGEMENT SYSTEM IN SUPPORT OF A GROUND WATER REMEDIATION PROGRAM

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ABSTRACT

During the period of 1978 to 1984, a medical materials manufacturing company used tetrachloroethylene (PCE) as part of its production process. In 1984, the company ceased operations and, during facility closure, hydrological testing revealed that significant amounts of PCE were present in the ground water and soils. The aerial extent of PCE in the ground water and unsaturated soils was determined to be approximately eight acres and one acre, respectively.

Remediation efforts over the past four years have generated a large quantity of monitoring data from various systems including: 58 ground water monitoring wells, 37 ground water recovery wells, 18 soil vacuum extraction wells, a ground water collection trench and a ground water recovery treatment system. Collection and interpretation of the data required the development of a data management system capable of handling large quantities of information. Data gathered during remediation includes: PCE concentrations in ground water, PCE concentrations in air extracted from unsaturated soils, ground water levels and vertical ground water flow gradients.

An important feature of the system is that it is user-friendly. The menu-driven program encourages clerical input and output while allowing for technical quality control and editing. The system is designed for one-time data entry, whereby data manipulation is performed internally through a selection of output options. Several tabular and graphical outputs are available. Graphing is performed through a user's-choice process to export data to various graphing packages.

The advantage of this package is that it can handle a variety of data parameters, stores them in one easy accessible location, outputs them in various user-selected formats, and is a menu-driven, user-friendly system. This system is currently being expanded for use on other environmental projects on a company-wide basis.

INTRODUCTION

In 1984 RMT, Inc., was retained during closure of a medical materials manufacturing company which used tetrachloroethylene (PCE) as part of its production process. Hydrological testing for facility closure revealed that significant amounts of PCE were present in the ground water and soils. Through further investigations, the aerial extent of PCE in the ground water and unsaturated soils was determined to be approximately eight acres and one acre, respectively.

Over the past five years, remediation efforts have generated a large quantity of data from various systems including: 58 ground water monitoring wells, 37 ground water recovery wells, 18 soil vacuum extraction wells, a ground water collection trench, a ground water recovery treatment system, and recently, an air injection well. Due to the large volume of collected data and repetitive calculations required for data interpretations, a data management system was developed to store, sort, and generate outputs from the data. Data gathered during remediation includes: PCE concentrations in ground water, PCE concentrations in air extracted from unsaturated soils, specific conductance of ground water, ground water recovery flow rates, ground water levels, and vertical ground water flow gradients.

A program was developed for the purpose of compiling and organizing the operational data. It was designed using the dBase III programming features. It is user-friendly and is operated by a system of menus. Options are available for entering new data, editing existing data, backing up files, searching records, exporting to graphics packages, and generating tabular report formats.

Currently the system is being expanded for use on other environmental projects within the RMT, Inc.

BACKGROUND

The remediation effort was set up in four stages. The first being the initial investigation and background data gathering. This resulted in background monitoring well information and soil parameters. The second stage, or interim remediation, consisted of installing seven ground water pumping wells which added flow rate parameters to the project. Then a ground water collection trench was installed, followed by vacuum extraction systems for remediating the unsaturated soils. The third stage was the full-scale remediation effort consisting of 32 manifold jet pump wells which yielded large quantities of data. It was during this stage that the data management system was developed. The fourth stage of remediation is site closure, which is currently underway.

During the early stages of remediation, the number of wells and parameters were easily handled by manual interpretation. However, as the project grew, it soon became quite cumbersome and tedious to handle monthly data manipulation manually.

PURPOSE

As stated previously, the data management system is a means of storing, sorting, and manipulating the data to the desired format, be it graphical or tabular output. Its main purpose is to perform repetitive manipulation of the data. The system is divided into several menu systems which allow the following tasks to be performed:

- Exit to DOS.
- Exit to Dbase.
- Enter new data.
- Edit existing data.
- Backup old file.
- Export to graphics.
- Generate reports.

Within these features, the data is used to calculate many other needed parameters. For example, running totals of pounds or gallons of PCE removed from the site. This assists the project coordinator by always having current totals available for planning and regulatory reporting.

OPTIONS

Through the seven options listed above, the program can be used to take raw input data and generate specific output needs. The first two options simply allow the user to exit the system, if necessary. One can exit back to the basic dBase COMnand center or exit the system all together and go back to DOS commands.

The third choice, enter new data, gets you into a submenu which specifies the type of information you may enter. The categories are as follows:

- Pumping wells.
- French drain pump.
- Jet pump system A.
- Jet pump system B.
- Vacuum wells.
- Collection trench.
- Air strippers.
- Vacuum trenches.
- Dual extraction wells.
- Discharge flume.
- Vacuum pumps.
- Stream gages.
- Piezometers.
- Fountain Inn Frozen Foods
- WCRSA
- Background wells.
- Monitoring wells.

These categories have a number of wells each of which has a file previously set up

with record and field information. Each category selection is a sub-program which allows the user to enter specific parameters (fields) for that particular category. For example, the pumping well files contain the following fields: PCE concentrations, specific conductance, flow rate, date, time, sampler, sampling method, temperature, meter reading, vacuum reading (inches of mercury), vacuum flow rate, air PCE concentration, and miscellaneous notes. They do not, however, contain a field for water level like the monitoring wells would, and the monitoring wells will not contain a field for meter readings or flow rate calculations.

The fourth option is editing any previously entered data. The user goes in to the same menu as was used for entering new data. A specific category is chosen and the values changed as needed. The changes are made by calling the field of interest and the date for which that field is to be altered (each field is tied to the main category and date). Next is the option of automatically backing up the data files the user is either currently in or those which have been opened, used, and need to be closed with new back up files created.

The last two options are the final usage stages of the entered data. First, data can be exported to a variety of graphics packages, these include the following:

- Lotus
- Freelance (by Lotus)
- Grapher
- Surfer

Currently, the user specifies which fields of a record are to be graphed, and the data is exported through ASCII. Data can then be imported into a graphing package. The graphing package used most often for this project is Grapher. Typical output from Grapher is shown in Figures 1 and 2. Figure 1 shows a semilog plot of PCE versus time for an individual well, and Figure 2 is a standard xy plot of water level elevations versus time. The final option is to generate reports.

The data management system provides for a variety of tabular output displays. These include the following the following:

Water levels

- quarterly
- historical

PCE tables

- historical

Specific conductance

- historical

Individual well flow rate

- quarterly
- historical

Individual well PCE removal

- quarterly
- historical

DATA MANIPULATION

Once the data has been entered, the different parameters are used in a variety of calculations to achieve the output forms. These calculations are built into the database system so that the user simply enters the raw data, and a multitude of things go on behind the scenes. Different data manipulation categories include the following:

- Water level calculations.
- PCE concentrations and specific conductance.
- Ground water flow rate calculations.
- PCE removal of ground water recovery.
- Vacuum extraction.

WATER LEVEL CALCULATIONS

Original depths to water were gathered for each well during installation. The original values were then input into the database as the original reference for the ground water

B-10A AND B-10B
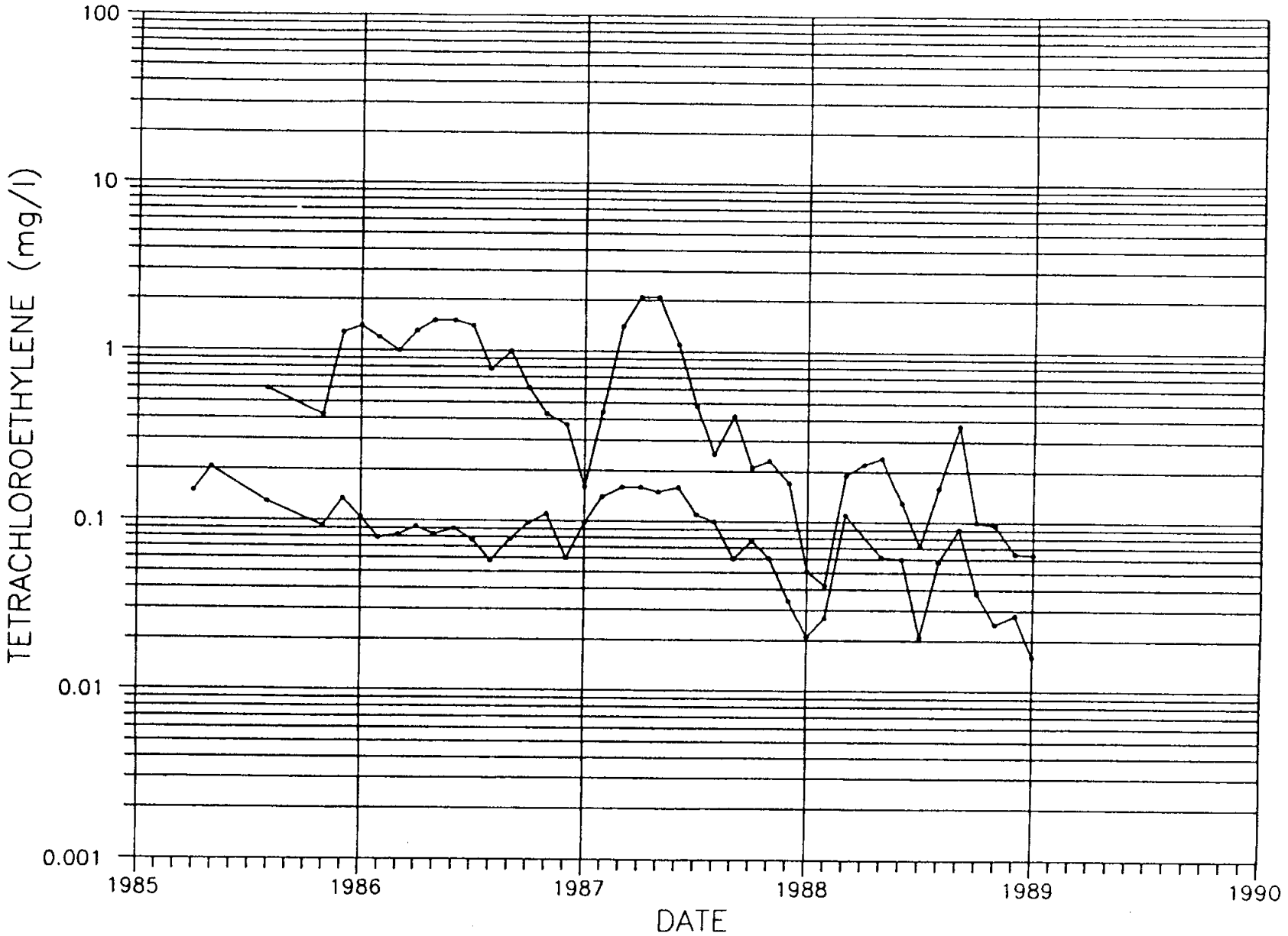TETRACHLOROETHYLENE VS TIME PLOT

FIGURE 1.

HYDROGRAPH

ELEVATION
(Feet Above Mean Sea Level)
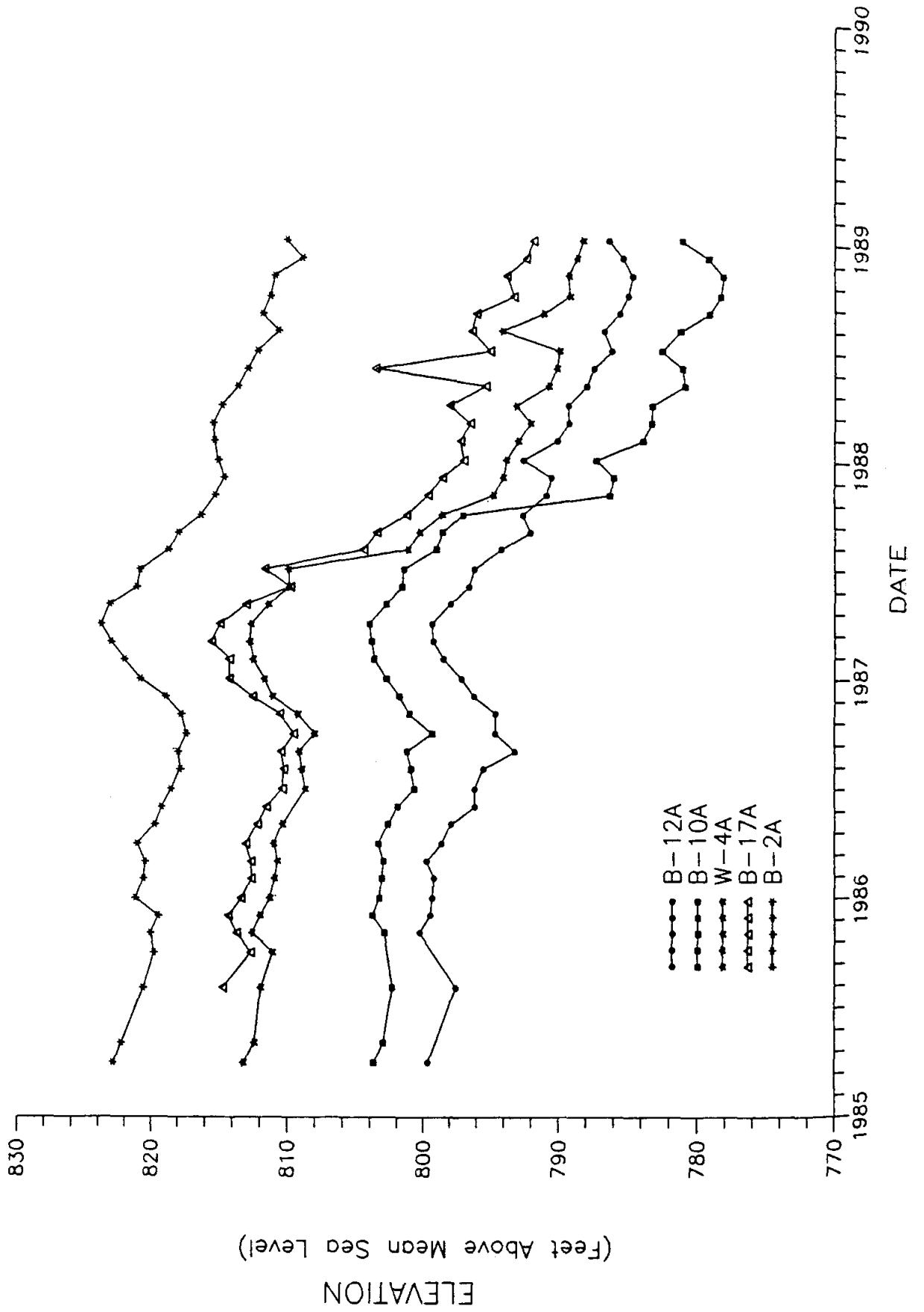
DATE

B-12A
B-10A
W-4A
B-17A
B-2A

table elevation. Over the years, monthly monitoring has been performed with each well's depth to water entered into the system. Also at the time of installation, the top of each well casing was surveyed to get the elevation above Mean Sea Level (M.S.L.). The monthly depth to water is then automatically subtracted from the top of casing elevation to arrive at monthly water table elevations.

SPECIAL INVESTIGATIONS

The database also has in it some special water level investigations. One set of data includes daily water level readings for all wells for a period of three weeks. This was a special study done last August to determine the rise in water level for various site areas, if all pumping systems were turned off. The second set of special data is for a select set of wells surrounding a newly installed air injection system. These special situations are noted here to emphasize that different forms of output are available: daily for all wells, daily for a select group of wells or the most often used historical (see Figure 3), and quarterly water level tables.

Water level information is also used to calculate vertical gradient between two wells. The vertical gradient and data fields are then exported and used in Grapher for display (see Figure 4).

PCE CONCENTRATIONS AND SPECIFIC CONDUCTANCE

Each month, ground water samples are collected from specific wells. Values of temperature and specific conductance are determined at the time of sampling, and septa vials filled with the ground water for shipment to the laboratory for analysis of PCE concentrations, Sampling is preformed in three time frames.

All wells are sampled in a single event annually. Second is quarterly sampling. During the first month of each quarter, a large number of wells, but not all, are sampled. For the remaining two months of each quarter, a smaller group of select wells are

sampled. Historical output of PCE concentrations and specific conductance tables are shown in Figures 5 and 6. These two parameters are currently set up to print only in a historical table, because it is the overall change in value which is of interest.

A special feature is incorporated with the data entry portion for these two parameters. It is a flag or notification statement which prints out after data entry to notify the user that the current value is higher, lower, or the same as the previous month's value. This was designed to iMnediately notify the user of the direction (up or down) that the PCE concentration and specific conductance values are going. For example, if a current value is higher than last month's value, the project coordinator may want to keep a close watch on a particular well so extra remediation may be performed in a particular area.

GROUND WATER FLOW RATE CALCULATIONS

All ground water pumping wells, air strippers, jet pump wells, dual extraction wells, discharge flumes, and the ground water collection trench are equipped with digital flow meters. Different wells and systems are read at specific times throughout the month to determine flow quantities in each system. Daily, monthly, and historical flow rate can be calculated.

The most often used flow rate expressions for individual wells are as follows:

- Gallons per day for the quarter.
- Gallons per minute for the quarter.
- Total gallons for the quarter.
- Average gallons per day for the history of the well.
- Average gallons per minute for the history of the well.
- Total gallons removed for the history of the well.

Cumulative (a total of all pumping systems) calculations are also preformed. These values are used in quarterly reports submitted to the state and include the following:

WATER LEVEL (Feet Above Mean Sea Level - MSL)

DATE	W-1	W-2	W-3	W-4	W-4A	W-4B	W-5	W-5A	W-6	W-7	B-1	B-2	B-2A	B-2B	B-3	B-4	B-5
4/85	817.66	826.93	814.82	813.48	813.19		818.29	818.17	814.11	816.77	827.26	824.71	822.87	822.23	827.39	822.07	818.29
5/85	817.00	826.53	814.31	812.81	812.44		812.57	817.10	818.54	816.47	825.76	823.90	822.30	822.33	826.01	821.32	817.46
6/85																	
7/85																	
8/85	815.74	824.28	813.46	812.00	811.96	813.06	815.95	815.86	816.63	815.24	824.91	822.11	820.64	820.78	824.39	819.95	816.29
9/85																	
10/85		823.55	812.64	811.08	811.09	811.11	815.19	814.96	816.01	814.41	823.51	821.51	819.79	819.88	823.59	819.10	815.28
11/85	816.71	824.13	813.81	812.83	812.61	812.56	815.89	815.79	817.11	815.47	824.21	821.46	820.09	820.43	823.89	820.02	815.99
12/85	817.22	825.57	813.89	812.00	812.01	812.01	817.34	817.19	819.31	816.23	822.39	821.94	819.49	822.26	825.55	821.30	816.94
1/86	816.61	825.43	813.14	811.18	811.29	810.28	816.23	816.01	817.56	815.32	824.46	822.90	821.19	821.38	825.58	820.44	816.22
2/86			812.99	810.88	811.00	810.94	815.94	815.59	817.26	815.09	823.99	822.23	820.63	820.75	825.06	820.08	814.66
3/86	816.04	824.79	812.62	810.74	810.76	810.74	815.51	815.31	816.85	814.74	823.85	822.11	820.49	820.62	824.89	819.92	815.54
4/86	816.38	825.02	812.82	810.97	811.01	811.03	816.06	815.87	817.37	815.12	825.08	822.62	821.06	821.10	825.26	820.39	815.93
5/86	815.44	824.29	811.96	810.27	810.41	810.27	814.98	814.74	816.35	813.98	823.48	821.62	819.76	819.92	824.34	819.50	814.83
6/86	814.94	823.68	811.48	809.66		809.72	813.79	814.03	814.88	813.63	821.96	821.09	819.24	819.29	823.71	818.76	814.43
7/86	814.12	822.79	810.65	808.73	808.75	808.79	813.37	812.99	814.18	812.36	822.49	820.37	818.54	818.50	822.93	817.99	813.46
8/86	813.61	822.17	810.78	809.32	809.03	809.01	812.90	812.69	813.51	812.49	821.33	819.69	817.89	817.91	822.16	817.57	811.42
9/86	813.99	822.05	811.03	809.25	809.24	809.21	813.14	812.99	814.05	812.85	821.26	819.61	818.05	818.13	821.96	817.84	812.09
10/86	813.13	821.53	809.92	808.06	808.09	808.13	812.26	812.04	813.03	811.72	820.88	819.11	817.44	817.34	821.53	816.97	811.34
11/86	813.94	821.78	811.05	809.36	809.31	809.32	813.09	812.91	813.86	812.77	821.06	819.31	817.80	817.88	821.67	817.68	812.18
12/86			812.91	811.27	811.15	811.11	814.78	814.88	816.44	814.78		820.39	818.96	819.23	822.54	819.29	814.91

FIGURE 3.

VERTICAL GRADIENTS BETWEEN WELLS W-4A AND W-4B

FIGURE 4.

301

302
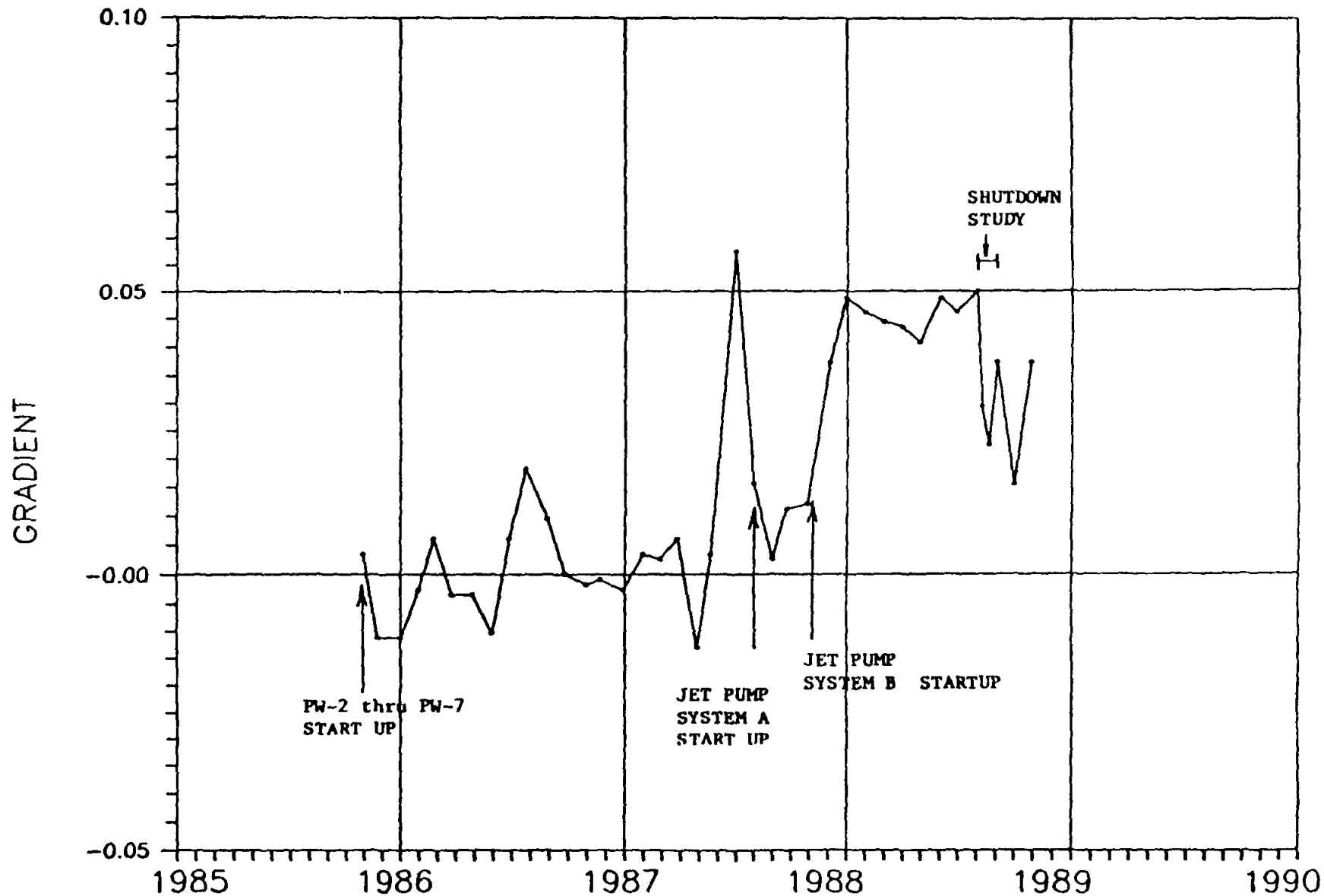
TETRACHLOROETHYLENE (mg/l)   Sampling Point

Date	W-1	W-2	W-3	W-4	W-4A	W-4B	W-5	W-5A	W-6	W-7	B-1	B-2	B-2A	B-2B	B-3	B-4	B-5
10/84		< 0.01	0.011	0.121			0.233		0.023	0.021	0.022	0.382			< 0.010		
11/84																	
12/84																	
1/85																	
2/85																	
3/85																	
4/9/85	< 0.01	< 0.01	0.020	0.169	29.5		0.159	0.153	0.032	0.014	0.206	1.64	< 0.010	< 0.010	< 0.010	0.090	0.251
5/6/85	< 0.01	< 0.01	0.018	0.165	19.9		0.241	0.084	0.023	0.015	0.042	1.127	< 0.010	< 0.010	< 0.010	< 0.010	0.283
6/85																	
7/85																	
8/19/85	< 0.01	< 0.01	0.018	0.131	15.4	27.2	0.182	0.051	0.020	0.014	0.471	0.412	< 0.010	< 0.010	0.011	< 0.010	0.471
9/85																	
10/85																	
11/5/85			0.015	0.183	15.6	26.9	0.073	0.060	0.018	0.034	1.960	0.552	< 0.010	0.047	< 0.010	< 0.010	0.339
12/3/85			< 0.01	0.183	19.3	29.7	0.103		0.032	0.055	0.395	0.552	< 0.010	< 0.010	< 0.010	< 0.010	0.351
1/6/86			0.010	0.233	23.4	39.2	0.087	0.057	0.031	0.089	0.456	0.506	0.018	< 0.010	< 0.010	< 0.010	0.363
2/4/86			< 0.010	0.177	20.8	35.2	0.084	0.070	0.012	0.078	0.788	0.281	< 0.010	< 0.010	< 0.010	< 0.010	0.611
3/4/86			< 0.010	0.240	24.0	39.0	0.097	0.089	0.010	0.130	1.400	0.310	< 0.010	< 0.010	< 0.010	< 0.010	0.550
4/1/86			< 0.010	0.240	12.0	36.0	0.080	0.063	< 0.010	0.100	2.00	0.380	< 0.010	< 0.010	< 0.010	< 0.010	0.460
5/8/86			< 0.010	0.320	18.0		0.068	0.048	< 0.010	0.092	3.00	0.180	< 0.010	< 0.010	< 0.010	< 0.010	0.440
6/4/86			< 0.010	0.290	26.0	33.0	0.081	0.036	< 0.010	0.250	1.80	0.160	< 0.010	< 0.010	< 0.010	< 0.010	0.400
6/24/86			< 0.010	0.210	25.0	29.0	0.081	0.026	< 0.010	0.094	1.90	0.076	< 0.010	< 0.010	< 0.010	< 0.010	0.380
8/5/86			< 0.010	0.170	13.0	32.0	0.110	0.034	< 0.010	0.082	0.690	0.074	< 0.010	< 0.010	< 0.010	< 0.010	0.500
9/2/86			< 0.010	0.099	8.0	26.0	0.083	0.025	< 0.010	0.051	0.500	0.130	< 0.010	< 0.010	< 0.010	< 0.010	0.280
10/6/86			< 0.010	0.160	6.2	26.0	0.130	0.025	< 0.010	0.056	1.10	0.160	< 0.010	< 0.010	0.014	< 0.010	0.330
11/4/86			< 0.010	0.120	4.7	22.0	0.130	0.029	< 0.010	0.044	0.960	0.040	< 0.010	< 0.010	< 0.010	< 0.010	0.290
12/3/86			< 0.010	0.075	5.3	28.0	0.072	0.044	< 0.010	0.046	0.680	0.096	< 0.010	< 0.010	< 0.010	< 0.010	0.250
1/6/87			0.013	0.079	3.7	25.0	0.035	0.028	< 0.010	0.014	0.084	0.057	< 0.010	< 0.010	< 0.010	< 0.010	0.170
2/3/87			< 0.010	0.051	4.9	32.0	0.041	0.039	< 0.010	0.021	0.057	0.130	< 0.010	< 0.010	< 0.010	< 0.010	0.190
3/10/87			< 0.010	0.031	3.2	31.0	0.040	0.090	< 0.010	< 0.010	0.071	0.068	< 0.010	< 0.010	< 0.010	< 0.010	0.220
4/13/87			< 0.010	0.120	4.8	20.0	0.068	0.055	< 0.010	0.018	0.099	0.130	< 0.010	< 0.010	< 0.010	< 0.010	0.210
5/5/87			< 0.010	0.084	5.4	14.0	0.077	0.073	< 0.010	0.014	0.110	0.260	< 0.010	< 0.010	< 0.010	< 0.010	0.200
6/1/87			< 0.010	0.074	8.5	26.0	0.120	0.110	< 0.010	< 0.010	0.440	0.300	< 0.010	< 0.010	< 0.010	< 0.010	0.150
6/30/87			< 0.010	0.061	6.8	22.0	0.150	0.120	< 0.010	0.013	1.10	0.430	< 0.010	< 0.010	< 0.010	< 0.010	0.120
8/3/87				0.05	4.5	15.0											
8/31/87				0.14	3.3	7.0											
10/9/87			< 0.010	0.12	2.1	4.4	0.47	0.160	< 0.010	< 0.010	1.20	0.100				< 0.010	0.059
11/4/87					0.98	3.6											
12/3/87					1.3	1.4											
1/6/88						1.9		0.065		0.031	0.093	0.024					
2/2/88					0.91	0.85											
3/1/88					0.58	0.76											
4/5/88					0.51	0.63		0.044				0.020					
5/88					0.56	1.5											
6/88					0.45	1.2		0.041				0.015					
7/88					0.38	1.1		0.035									
7/26/88					0.035	1.3		0.037									
8/22-9/1/88	< 0.001	< 0.001		< 0.001	0.470	2.1		0.022					< 0.001	0.620	< 0.001	< 0.001	
10/4-5/88					0.560	2.0								1.200			
11/14-16/88					0.500	2.0							< 0.001	0.660			
12/6-8/88					0.600	1.3							< 0.001	1.300			
1/4-5/89					0.770	1.2		0.041					< 0.001	0.980			

FIGURE 5.

SPECIFIC CONDUCTANCE (umhos/cm @ 25°C)
Sampling Point

FIGURE 6.

- Average gallons per day for the quarter.
- Average gallons per minute for the quarter.
- Total gallons removed for the quarter.
- Average historical gallons per day.
- Average historical gallons per minute.
- Total gallons removed for the history of the site.

Figure 7 shows both the quarterly and cumulative flow rate calculations described above. Tables of this format assist a project coordinator in determining flow quantities removed when reporting to regulatory agencies and to also assist in locating trouble areas. For example, when the total gallons value is small, there is most likely a problem with the pumping system, and it should be looked at as soon as possible.

PCE REMOVAL BY GROUND WATER RECOVERY

When the results of PCE concentrations are returned from the laboratory, the results are entered into the database. Using the number of gallons of water removed for that time period of sampling and the PCE concentration values, the number of pounds and gallons of PCE removed for each pumping system can be determined. These are reported in table form (see Figure 8). Figure 8 gives the number of pounds and gallons of PCE removed for each particular pumping system, as well as a running total.

Monthly and historical values can be reported for.

- Pounds of PCE removed for individual wells.
- Gallons of PCE removed for individual wells.
- Cumulative pounds of PCE removed.
- Cumulative gallons of PCE removed.

VACUUM EXTRACTION

During the investigation stage of the project, leaching tests were preformed on soils of three areas. The leaching studies revealed long-term leaching characteristics of PCE from the unsaturated soil zone. A soils remediation options analysis was preformed and a vacuum extraction system was selected. This resulted in further data to be evaluated.

Wells connected to the vacuum system were also ground water pumping wells so the system was two fold. When vacuum was applied to the wells, it not only stripped the PCE from the unsaturated soil, but it also assisted in ground water recovery by elevating the water levels. Monthly, the air flow rates and PCE concentrations are recorded for each well connected to the vacuum pump. A composite value is also read for each pumping unit. Again, calculations are done to determine the number of pounds and gallons of PCE removed via vacuum extraction as showm in Figure 9. Vacuum extraction parameters and calculations include the following (see Figure 10):

- Flow rate for pumping units.
- Flow rate for individual wells.
- PCE concentration per pumping unit.
- PCE concentration per individual well.
- Pounds of PCE removed per pumping unit.
- Cumulative pound of PCE removed.

SUMMARY

The database system was designed to handle a variety of data parameters, store items for different uses, and sort them in user-defined ways. The parameters are used to calculate flow rates for individual wells, as well as keep running totals of the number of gallons of ground water discharged from the site. It calculates the amount of PCE removed from the site both by ground water recovery and vacuum extraction. However, its biggest attribute is in the number of possible output formats the data can be displayed. Graphical output can be specified at any time, and a number of tabular formats are predefined to be selected for printing. One of the main features of the tabular output is the internal updating of cumulative sums. These cumulative sums are for flow volumes and PCE removal quantities.

	Flow for Reporting Period[1]			Cumulative Flow		
Recovery System	Total Gallons	Average GPD	Flow GPM	Total Gallons	Average GPD	Flow GPM
PW-1[2]	16	0.2	0.0	173,061	134	0.1
PW-2[3]	18	0.2	0.0	763,806	691	0.5
PW-3	596	6.8	0.0	567,695	513	0.4
PW-4	0	0	0.0	930,256	841	0.6
PW-5	484,305	5,503	3.8	5,745,285	5,195	3.6
PW-6	106,957	1,215	0.8	5,902,262	5,337	3.7
PW-7	113,296	1,287	0.9	1,604,406	1,451	1.0
Collection[4] Trench	373,013	4,239	2.9	8,959,509	12,091	8.4
DE Wells[5]	28,246	321	0.2	415,875	1,053	0.7
VE-1[6]	87,921	999	0.7	393,455	1,249	0.9
VE-3	0	0	0	147	0.7	<0.1
VE-9[7]	188	2.1	0	20,073	47	<0.1
PW-32[8]	205,665	2,337	1.6	1,137,725	3,366	2.3
PW-33	384,091	4,365	4.1	2,106,286	6,232	4.3
PW-34[9]	187,741	2,133	1.8	387,366	2,376	1.7
System A [10]	2,610,594	29,666	38.5	24,657,992	55,914	38.8
System B [11]	2,490,750	28,304	30.2	13,564,990	37,891	26.3
Totals	7,073,397[12]	80,384	89.2	67,330,192[13]		

(1) August 1, 1988 through October 27, 1988 (88 days).
NOTE: Flow averages are based on the entire reporting period. However, actual rates are higher since all recovery systems, excluding the collection trench, were shutdown for approximately 3 weeks in August.
(2) PW-1 Started April, 1985 (1292 days).
(3) PW-2 through PW-7 started October 15, 1985 (1106 days).
(4) Collection Trench Started on September 11, 1986 (741 days).
(5) DE Wells started on October 1, 1987 (395 days).
(6) VE-1 and VE-3 started on December 8, 1987 (315 days).
(7) VE-9 Started on August 21, 1987 (431 days).
(8) PW-32 and PW-33 started on November 24, 1987 (338 days).
(9) PW-34 started on May 18, 1988 (163 days).
(10) Jet Pump System A Started August 11, 1987 (441 days).
(11) Jet Pump System B Started November 4, 1987 (358 days).
(12) Note that the collection trench was the only recovery system operated during the shutdown study in August.
(13) The cumulative flow-total gallons in the previous quarterly monitoring report should have read 60,256,795 gallons instead of 60,616,800 gallons. This change has been incorporated into this report.

FIGURE 7.

Vacuum Pump	Tetrachloroethylene Removed For Reporting Period (1)		Cumulative Tetrachloroethylene Removed	
	Pounds	Gallons	Pounds	Gallons
V-1	281	20.8	5538[2]	409.4
V-2	553	40.9	3773	278.8
V-3[3]	2	0.2	197	14.6
Totals	836	61.9	9508	702.8

(1) August 1, 1988 through October 31, 1988 (96 days).

(2) Includes 1290 pounds removed during pilot demonstration from October 14, 1986 through November 9, 1986 performed on wells VE-1, 2, 3, and 4.

(3) Vacuum pump V-3 was discontinued on August 12, 1988.

FIGURE 8.

Recovery System	PCE Removed for Period Nov. 1988 through Jan. 1989		Cumulative PCE Removed	
System	Pounds	Gallons	Pounds	Gallons
PW-1	<0.1	<0.1	3.6	0.4
PW-2	<0.1	<0.1	14.7	1.1
PW-3	0.1	<0.1	5.5	0.5
PW-4	<0.1	<0.1	10.4	0.8
PW-5	26.5	2.2	1,034.8	76.5
PW-6	0.1	<0.1	846.5	62.6
PW-7	1.5	0.1	115.8	8.7
Collection Trench	0.2	<0.1	23.3	1.7
DE Wells	<0.1	<0.1	0.5	<0.1
VE-1	0.9	0.1	43.6	3.3
VE-3	0	0	<0.1	<0.1
VE-9	0	0	23.0	1.7
PW-32	0.1	<0.1	0.4	<0.1
PW-33	0.7	<0.1	9.4	0.7
PW-34	20.8	1.5	61.8	4.6
PW-35	26.7	2.6	26.7	2.0
System A	21.6	1.6	469.4	34.7
System B	12.5	0.9	94.6	7.0
Totals	112.0	9.0	2,784.2	206.3

FIGURE 9.

Month/Year	Estimated PCE (ppm)	Cumulative PCE (lbs.)	Pump Hours
November 1986	144-31	528.62	411
December 1986	157-14	405.81	584
January 1987	101-30	178.34	381
Febuary 1987	30-22	140.12	483
March 1987	23-9	161.94	850
April 1987	39	184.47	407
May 1987	39-35	292.87	690
June 1987	35-26	197.2	499
July 1987	26-22	145.84	555
August 1987	22-20	83.64	350
September 1987	20	148.1	648
October 1987	51-20	286.98	684
November 1987	43-17	223.05	672
December 1987	15.7-10	129.3	840
January 1988	24.3-7.1	106.02	658.5
Febuary 1988	25.7-18.6	138.17	628.5
March 1988	23-12.7	225.37	1055
April 1988	23-11.4	37.32	309
May 1988	18	127.76	670
June 1988	15	97.25	612
July 1988	18	127.76	670
August 1988	12	87.63	707
September 1988	14.3	76.35	504
October 1988	16	116.84	707
November 1988	12	84.78	684
December 1988	8.3	62.17	707
January 1989	11	78.08	670

FIGURE 10.

The database was originally designed for the specific ground water remediation project described. However, it is now being altered to be more of a general system to handle a variety of RMT's projects. It is currently being adapted for the following:

- Additional wells - to be added as needed.
- Other parameters - as needed.
- Better search and sort techniques.
- Varied output - both graphical and tabular.
- Better communications between graphics packages.

MANAGING DATA FROM A LARGE-SCALE GROUNDWATER MONITORING PROGRAM

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INTRODUCTION

The Savannah River Site (SRS), which has been in operation since 1952, is a 320-square mile reservation that produces plutonium and tritium for the national defense program. As a result of past waste handling practices the groundwater at several locations at SRS has become contaminated with solvents, metals and radionuclides. In 1981 the groundwater located under the Site's fuel and target rod fabrications area (M-Area), was found to be contaminated with degreasing solvents, primarily trichloroethylene and tetrachloroethylene. The total inventory for these solvents in the groundwater has been estimated to be 500,000 pounds. Since this contamination was detected over 270 monitoring wells have been installed in this area to assess the vertical and horizontal extent of the plume. In September of 1985 an air stripping column, designed to treat 400 gpm of water, was placed into operation. Since 1985 over 700 million gallons of groundwater has been treated. Approximately 180,000 pounds of degreasing solvents have been removed from the groundwater. The groundwater clean-up program in this area is expected to continue for 30 years.

Over the past several years attention to environmental issues has grown, which has resulted in laws that are designed to protect the environment. Groundwater protection has been the focus of part of the legislation and has been receiving more attention by the public. The groundwater protection program at SRS, in response to these influences, has grown dramatically. In the past ten years the number of groundwater monitoring wells has grown from 200 to approximately 1000 (Figure 1). The site currently has approximately 60 professionals dedicated to the protection and restoration of this valuable resource.

The purpose of the paper is to describe how the SRS groundwater data management system is used to verify, manipulate, and store groundwater data and how it is used to fulfill regulatory requirements. This paper will describe the development of the M-Area groundwater data management program and will focus on how the well, field and analytical data from this program are managed.

DESCRIPTION OF MONITORING PROGRAM

Sitewide Groundwater Program

The policy of the Savannah River Site (SRS) is to prevent or minimize degradation of natural resources and to take restorative action should such degradation occur. The

purpose of the Site's groundwater program is to detect and to quantify any degradation in groundwater quality. The program also supports research in conjunction with the Savannah River Laboratory (SRL).

The SRS groundwater monitoring program consists of radioactive and nonradioactive sampling and is operated by the Health Protection Section (HPS). The radioactive monitoring program began in the early 1950's and primarily monitors for gross radiological parameters at selected sites.

Groundwater monitoring for nonradioactive constituents began in 1975. All wells in this program are sampled either quarterly or biannually. The samples are analyzed by laboratories which are certified by the South Carolina Department of Health and Environmental Control (SCDHEC). It is estimated that approximately 90,000 laboratory analyses will be performed on SRS groundwater samples in 1989.

M-Area Groundwater Program

The M-Area groundwater program began collecting quarterly groundwater samples in 1983. The purpose of the sampling program was to: 1) Delineate the vertical and horizontal extent of the solvent plume; 2) Design an effective remediation program and 3) Meet regulatory requirements promulgated by the Resource Conservation and Recovery Act (RCRA). The same monitoring program is currently used to determine the effectiveness of the corrective action program. Due to the large quantity of data that was expected to be generated over the life of the project a computer based data management program was developed. The system is designed around the Statistical Analysis System (SAS) programming language which is resident on a IBM 3081 mainframe computer.

To make the M-Area groundwater program more efficient the duties of sample collection and initial data review are centralized in the Site's HPS. However, M-Area personnel are responsible for scheduling activities, data analysis, report generation and program upgrades.

Program Description

The M-Area groundwater program consists of several interdependent subprograms as shown in Figure 2. The success of the entire program requires that each subprogram operate efficiently. As can be seen from this figure the database management system is an integral part of the program. It is important that the database manager be familiar with the groundwater program and have an understanding of groundwater flow, contaminant transport and the operation of micro and mainframe computers.

Remedial action selection and implementation was based on hydrologic, geologic and analytical data collected in the field. The modeling of these data helps predict the effects of the remediation program and was initially used to help site the recovery wells which feed the production air stripping tower.

By law, SRS is required to prepare a quarterly groundwater corrective action report. This report, which must contain the field, hydrologic and analytical data, is due to SCDHEC for review thirty days after the close of the quarter. Also required as part of the report are analytical data posting maps, piezometric maps for each water bearing unit and a statistical data analysis designed to determine trends. The purpose of the report is to determine the effectiveness of the remedial action program.

System Description

The M-Area database management program is centered around the IBM 3081 mainframe computer. All well, field (including and stored on this system. For ease of retrieval and for optimal merging the data from the program are stored in three distinct files. They are the well data, field data (includes hydrologic data) and analytical data files. Each well has only one well data record and it contains information about the well which does not change (location, screen zone, top of casing elevation, etc). The field data is a single record of data that is recorded each time the well is sampled. A field data record contains such information as date, time, pH, water temperature, conductivity, etc. . For each field data record

Increase in Monitoring Wells

Increase in Analyses
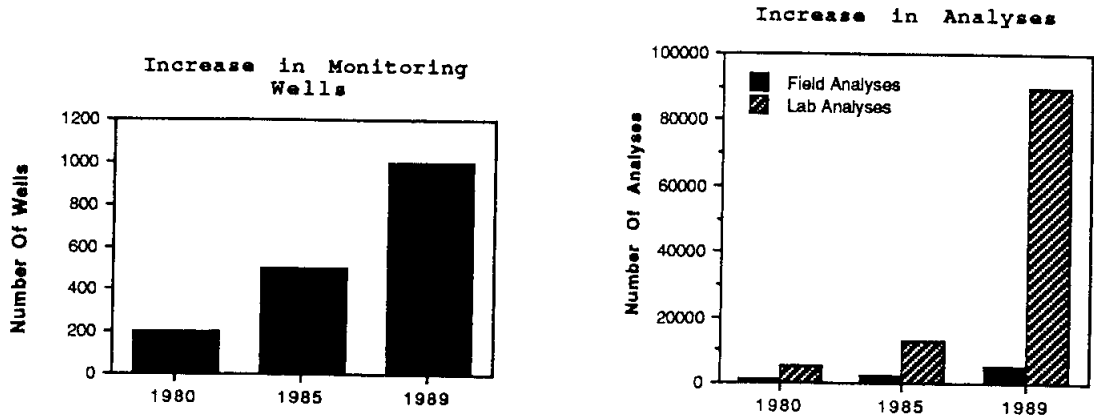
FIGURE 1
PROGRAM GROWTH
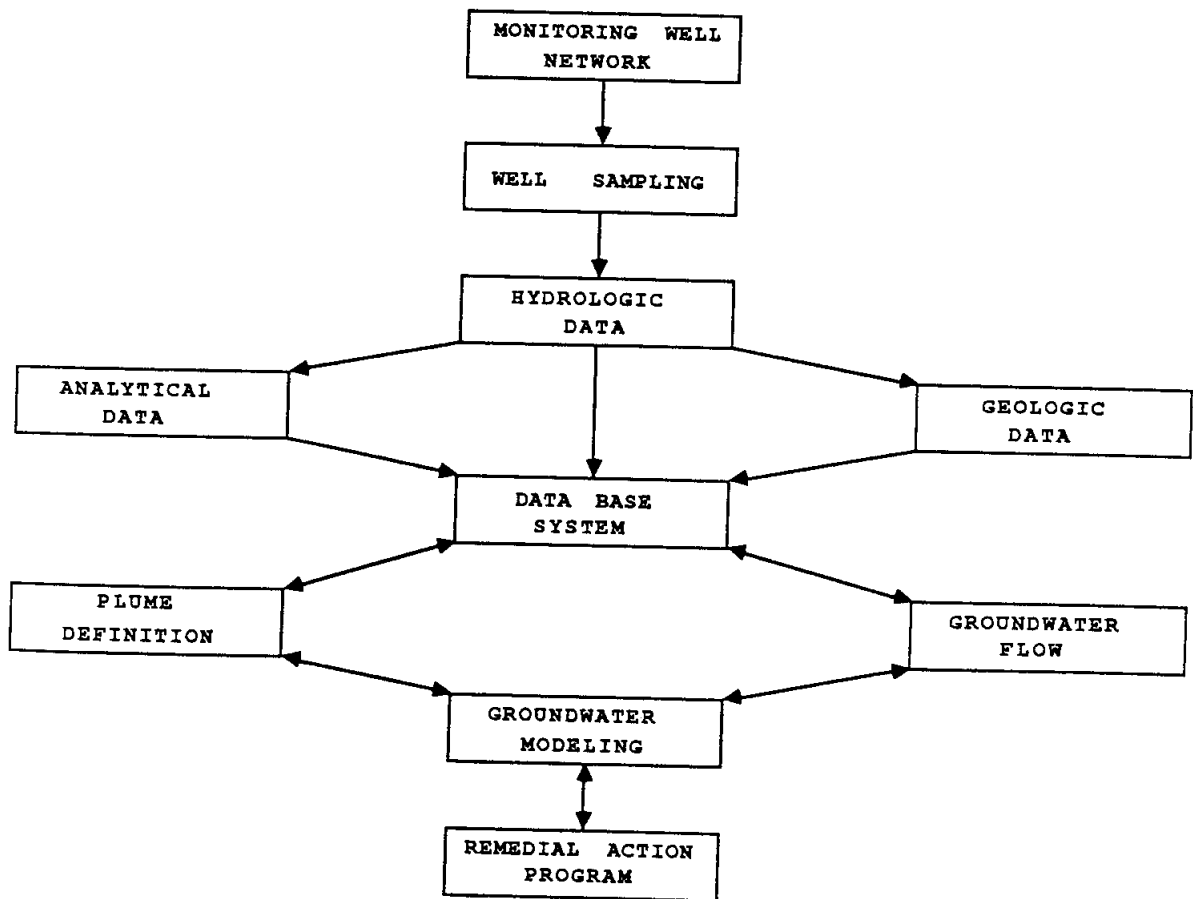
FIGURE 2
PROGRAM FLOW

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there can be one to many analytical data records depending on the type of analysis being performed. Each analytical data record contains the results for a specific constituent. The relationship between the well, field and analytical data is shown in Figure 3.

DATA COLLECTION, TRANSCRIPTION, TRANSFER AND STORAGE

Data Collection

The success of the groundwater program depends on the quality of the data. It is, therefore, very important that qualified personnel collect this information. The sampling personnel at SRS are required to have prior groundwater sampling experience and be trained to follow a standard protocol. This protocol, developed specifically for SRS, is entitled Hydrogeologic Data Collection and also includes standards for well installation and data handling.

Quality assurance is an important part of the groundwater program and includes the use of blanks and chain of custody procedures. To better manage the sampling program the computer is used to generate chain of custody forms that list the number and type of sample to be collected from each well.

Data Transcription

All data collected in the field are transcribed to a data coding form which is later used to enter the data to a floppy disk. A field data log book is also kept which is used to record daily events. The log book is verified each day, signed and witnessed. The completed field data sheets and field log book are kept as permanent records. Figure 4 shows how data are entered into the Site mainframe computer. Well data are keypunched directly into the appropriate file on the mainframe. All field and hydrologic data are keypunched and saved as ASCII files on IBM PC compatible disks. The software used to save the data is written in BASIC and is designed to check the data as it is entered for correctness.

Analytical data generated by the on-site analytical laboratory are uploaded to the Site's mainframe computer via the Local Area Network (LAN) and then review by laboratory personnel prior to release. These data are stored on disk as flat ASCII files prior to permanent storage on nine track tape as SAS formatted files. Prior to permanent storage the data are reviewed by M-Area personnel both visually and by computer. Any data which is suspect is verified before being added to the master tapes. Analytical data received from off site laboratories are sent on floppy disk as flat ASCII files in a specified format. Laboratory Information Management Systems (LIMS) are used to load these data to microcomputers which create IBM PC compat-ible ASCII files. The use of this type of system helps eliminate transcription errors.

Data Transfer

All data that is keypunched or loaded to disk via LIMS are transferred to the Site's mainframe computer using a commercial software package known as PCLink. Each type of data is sent to a predetermined location as shown in Figure 5. All data are then visually and software reviewed prior to final storage.

Data Storage

As described earlier all data collected as part of the groundwater program are stored on the IBM 3081 mainframe computer either on disk or tape as ASCII or SAS files.

Analytical data are backed up using a "Round Robin" approach which is illustrated in Figure 6. The system consists of nine nine-track tapes. Data sets are added to each tape sequentially beginning with tape LA 3425 while new data are always added to tape LA 3440. Using this approach there are always two tapes available with the most current data. Once tape eight (LA 3432) is completed the next update writes over tape LA 3425 and the process begins again. A log of the updating process is stored as a separate file. To protect this tape backup system only tape LA 3440 is made available for general Site use.
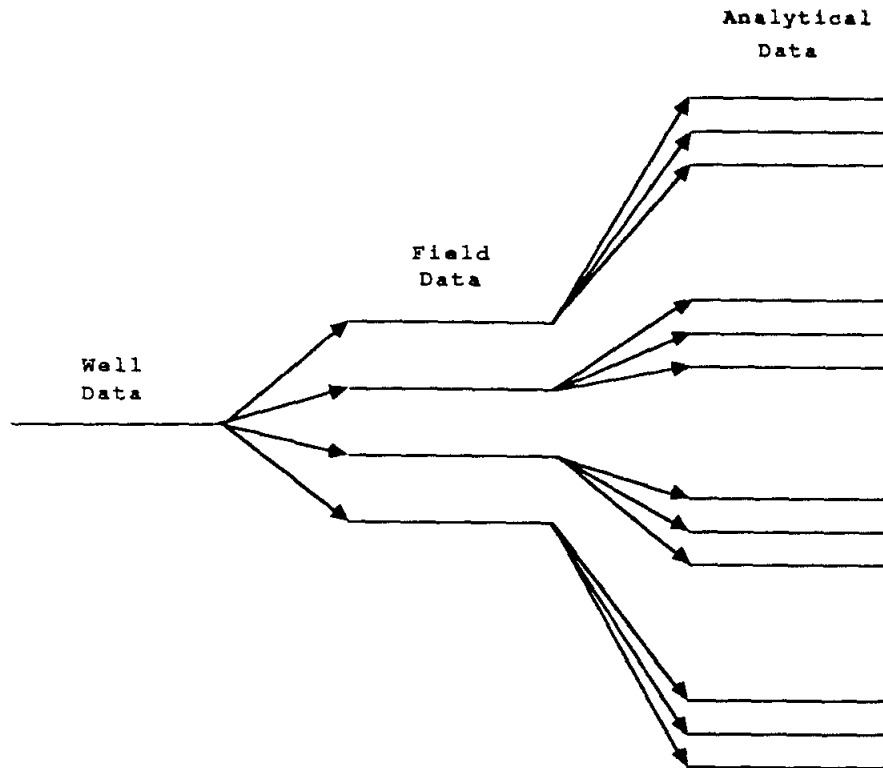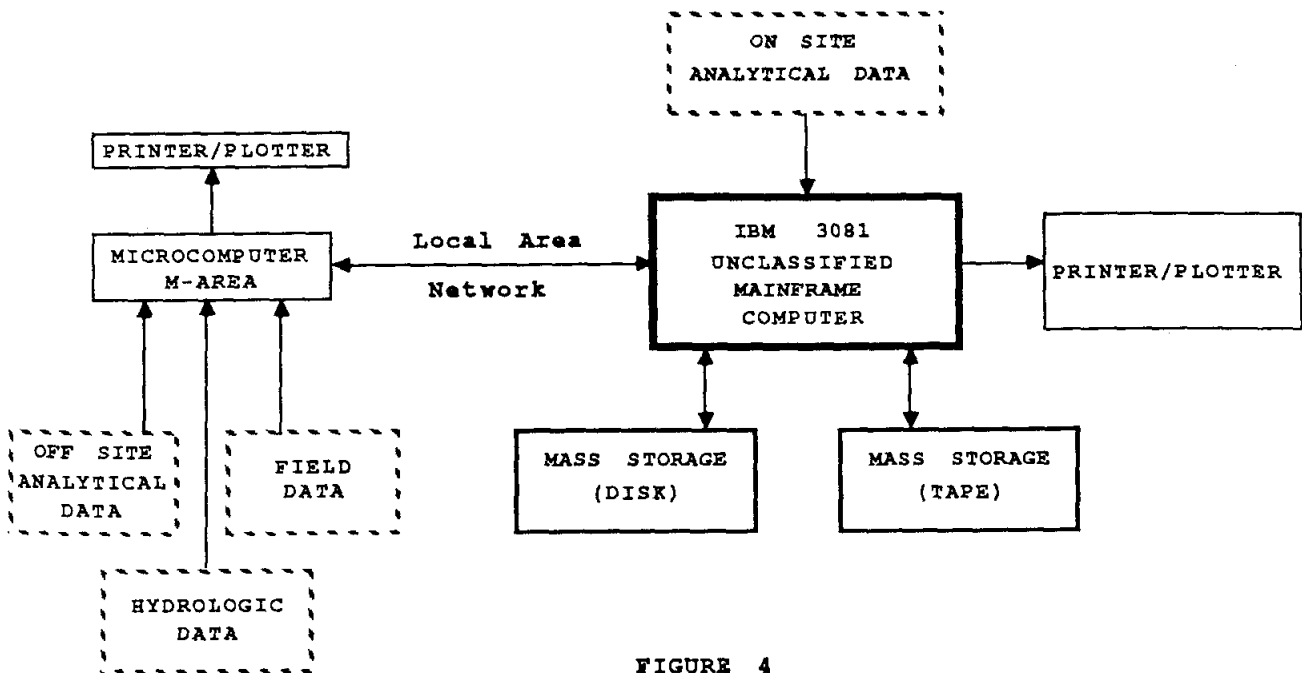
FIGURE 3

DATA RELATIONSHIP
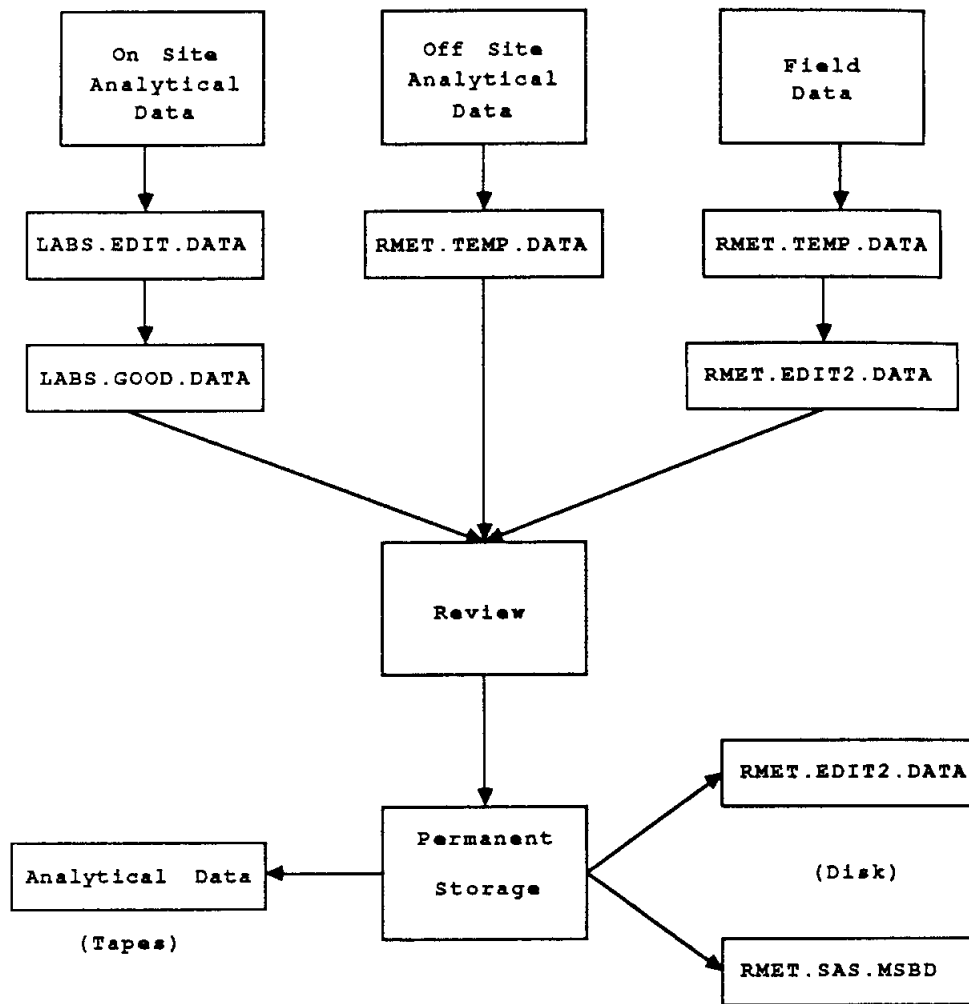

FIGURE 4

DATA FLOW DIAGRAM
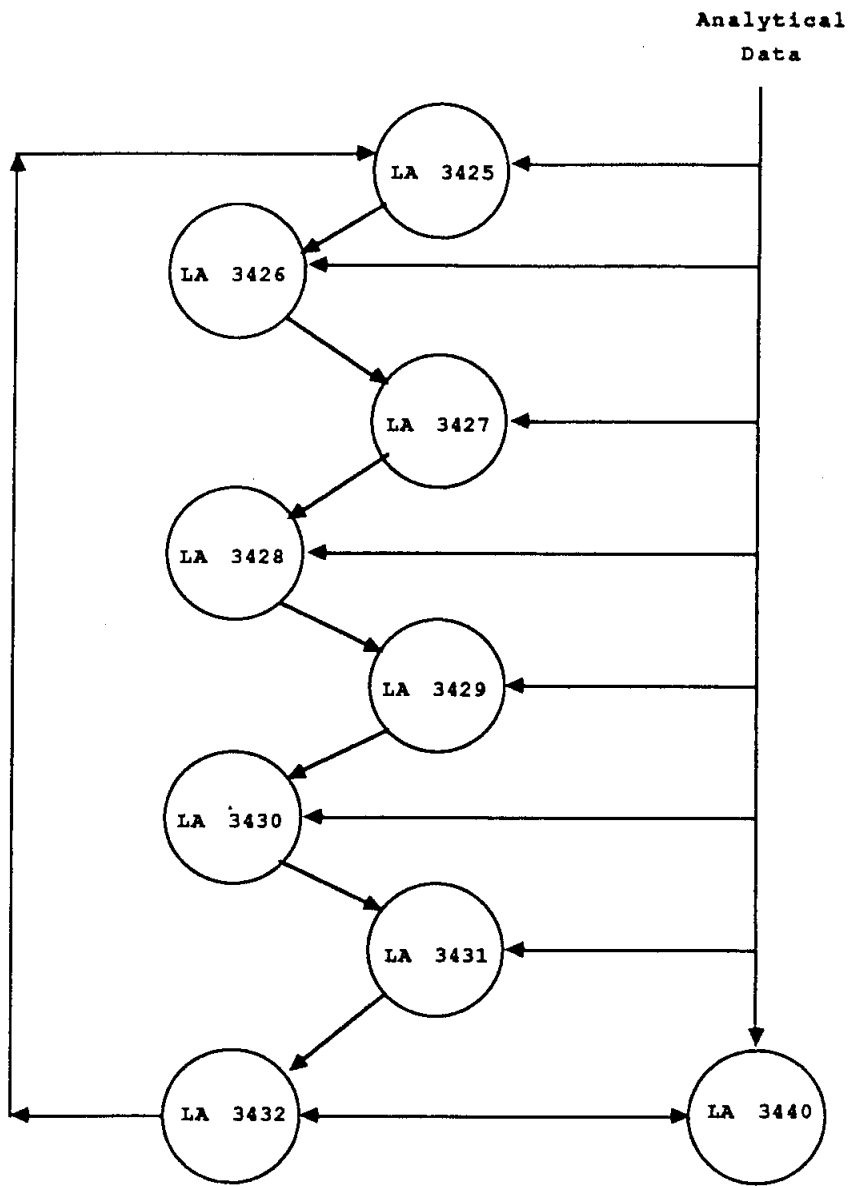
313

Figure 5
Computer Data Flow

314

FIGURE 6

Analytical Data Storage and Tape Backup System

315

Data and software are also stored on high-volume disk drives as flat ASCII or SAS files. Figure 7 is a block diagram showing each storage location and its intended purpose.

Data Manipulation

To fulfill the requirements of the M-Area corrective action report several programs have been written in SAS to produce the required data tables, hydrographs and time/concentration plots. To analyze the trends in the analytical data a Cumulative Sums (CUSUM) technique is used. Since this analysis is better done in an interactive environment the necessary data are downloaded to an IBM PC/XT microcomputer and analyzed using a BASIC program.

The piezometric and data posting maps are produced using PC ARC/Info, a Geographic Information System (GIS), written and sold by Environmental Systems Research Institute (ESRI). Since the PC version of this software can not create contours a commercial package entitled SURFERTM by Golden Software is used. The output from this package is converted, using a special algorithm, to the proper ARC/Info format and is then plotted over the area base map using ARC/Info. The ARC/Info GIS is both a powerful and flexible tool allowing editing of the final product. By using SURFERTU to create the piezometric contours the data are analyzed the same way each quarter allowing for a more meaningful quarter to quarter comparison.

The use of the Site mainframe, and the commercial software packages (SURFERTU and ARC/Info), allows SRS to produce the quarterly corrective action report in the allotted thirty day period thus meeting the requirements of the Site's RCRA permit.

FUTURE PLANS

Recently the need for good quality environmental data, that is accessible to all users, was identified. As a result of this need a Sitewide Environmental Data Management Committee was formed. One mission of the group is to identify all existing environmental databases at SRS and transfer them to a central computing facility. The relational database ORACLE was selected as the data manager and will eventually reside in a large-scale VAX environment. The groundwater data was selected to be the first information that will be entered into the system. A transparent interface is also being developed that will allow for a user-friendly way to access these data.

A sitewide GIS is also being developed and the USGS 7.5 minute quadrangle sheets that comprise the site are being digitized for use as base maps. The GIS will be used in conjunction with the ORACLE database to better manage, manipulate and output the groundwater data from SRS.
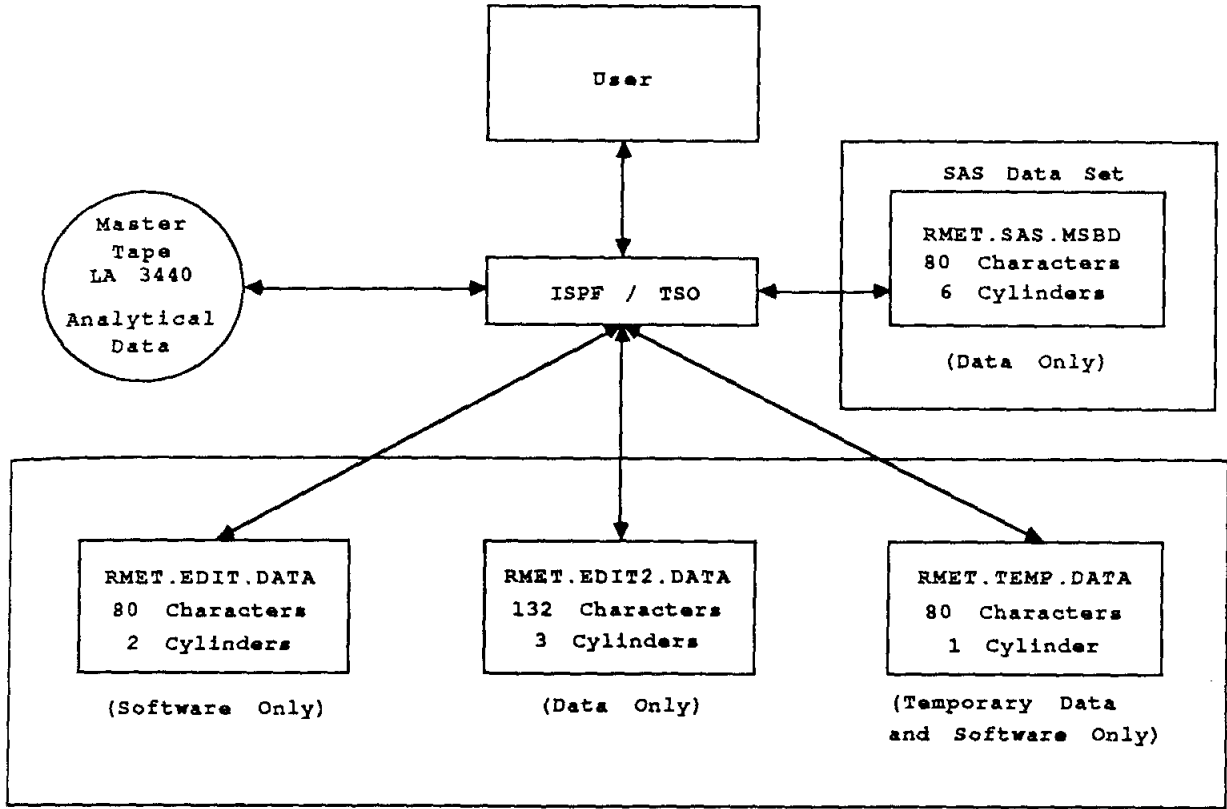
Figure 7
Data Storage Diagram

COMPUTERIZED URBAN RUNOFF WATER-QUALITY DATA HANDLING BEGINS WITH ELECTRONIC DATA COLLECTION AND LABORATORY REPORTING

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and

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INTRODUCTION

The quality and quantity characterization of urban storm runoff is necessary for assessing, planning and designing facilities to reduce the impacts on receiving waters. Typically, data collection includes the measurement of both streamflow and water quality at multiple points on a storm runoff hydrograph (Fig. 1) in order to obtain design loadings for runoff treatment facilities. Event mean concentrations (EMC), as proposed by the U.S. Environmental Protection Agency (1983), may be calculated from the type of hydrograph sampling shown on Fig. 1. Collecting, handling, analyzing and reporting of water quality and discharge data in an urban runoff monitoring network is facilitated by specialized computer-based data collection techniques. Manually entering stage data or water-quality values into a spreadsheet or other computerized data management system could easily become prohibitive from both a time and data transcription standpoint. This paper discusses how data may be collected electronically in the field and received electronically from the analytical laboratory and then analyzed and reported using computer-based data collection and reporting methods. A field example deals with collection and analysis of data in the Cherry Creek basin in the Denver metropolitan area, Colorado (In-Situ Inc., 1989; Kunkel, 1988;

Steele and Wemmert, 1988; Steele and others, 1989). Examples of output of basic statistics, water-quality variables, nutrient loads, daily mean discharge, regression analysis, and data reporting also are given.

ELEMENTS OF AN ELECTRONIC DATA COLLECTION SYSTEM

The rapid development of the microchip and microcomputers within the last few years has resulted in the availability of powerful data loggers, samplers and other computer hardware for collecting data and automatic water sampling at remote sites. The major elements of a typical urban runoff water quality data collection system might include a data logger and automatic water sampler, selected computer hardware for transferring data from the field to the office, obtaining laboratory data in digital form, and a computer software structure to reduce and analyze the field data.

The objective of the electronic data collection system is to minimize the introduction of errors associated with manual data entry as well as reducing field and office time associated with the transfer of raw data into a usable form. Each of the elements of a typical electronic data collection system for urban runoff water quality data handling is detailed below.
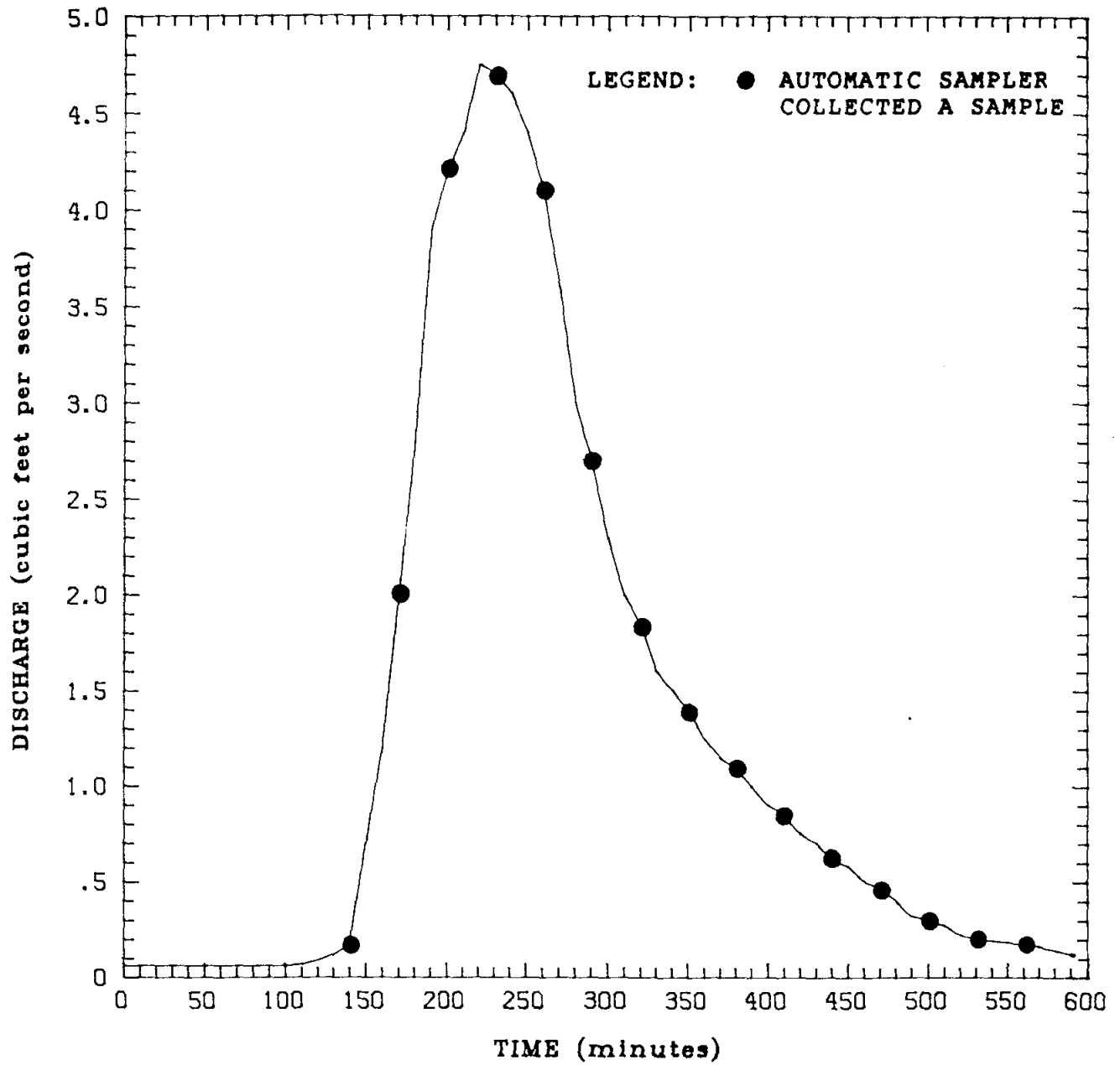
318

Fig. 1   Storm Runoff Hydrograph and Times when a Water-Quality Sample was
Collected

Data Logger and Sampler

The two aspects of an urban runoff water quality data collection system are (1) the measurement of continuous stream stage, and (2) the collection of discrete water-quality samples during extreme rainstorm and snow-melt runoff events. A typical water-discharge and water-quality sampling installation is shown on Fig. 2.

In an urban setting, runoff hydrographs often reach their peak discharge after several minutes because of the generally short times of flow concentration and small watershed areas. In order to accurately represent a typical urban storm runoff hydrograph, a time-discharge relationship consisting of stage measurements recorded at five to ten minute increments is usually needed. Therefore, a typical data logger should be capable of collecting data at intervals of at least every five minutes and storing data at five minute intervals for up to one month prior to data transfer. This would require that up to 8,000 time-stage data pair values be stored in the data logger. An alternative to storing large numbers of data points would be to have a programmable data logger which would be actuated to begin data collection at a preset stream stage so that only the storm runoff hydrograph data were collected with ambient or low flow data ignored as part of the data collection program.

The automatic water sampler should be capable of collecting a sample at a prespecified stream stage or discharge, and also capable of taking a sample at preselected time intervals over the storm hydrograph. Our recommendation is that the best method for obtaining "representative" water-quality samples which may be used to estimate an EMC is to collect samples at equal time increments and then composite them by hand based upon the actual storm hydrograph. This recommended procedure requires that the time between samples be short enough to obtain representative samples over the complete storm hydrograph. Because most automatic water samplers are limited to 24 bottles once the sampler is actuated, some skill in knowing what time intervals to program between samples is required to insure sampling over

the runoff hydrograph. We also recommend that the automatic water sampler be actuated at a preset stage by the data logger so that the exact time when the sampler begins sampling will be known from the time and stage data stored in the data logger. Alternative automatic water sampler actuator devices also are available. These actuators generally consist of two wires suspended above the water surface. When the water surface rises to a certain level, the two wires are submerged completing an electrical circuit which tells the automatic sampler to begin sampling at the prespecified stage intervals; however, we believe that compositing samples based upon stage or a prespecified hydrograph does not accurately reflect urban runoff conditions for characterizing water quality.

Computer Hardware

The computer hardware components for a computerized urban water quality data collection system at a given site might consist of the items shown schematically on Fig. 3. The cost of such a system might include up to $4,000 for a data logger and pressure transmitter to collect time and stream stage data which then would be converted to instantaneous time and discharge data; up to $2,000 for an automatic water sampler; up to $3,000 for a laptop computer; and up to $6,000 for a microcomputer. The data logger time and stream stage information values could be transferred to either the laptop portable computer in the field or to a microcomputer in the office using a standard RS232 interface. Peripheral plotters and printers for the microcomputer may cost up to $2,000 each, depending on the options desired. The advantage of transfer of data electronically includes reduction of time-consuming hand compilation of data and minimization of errors in transferring the data.

Laboratory Water-Quality Data

Generally, water-quality samples of urban runoff are analyzed for more than one chemical constituent. Typical water-quality variables which may be analyzed for each sample might include nutrients, suspended sediment, selected trace metals, and possibly major anions and cations for selected samples.

AUTOMATIC WATER SAMPLER   LOCKED BOX

DATALOGGER

PRESSURE
TRANSMITTER
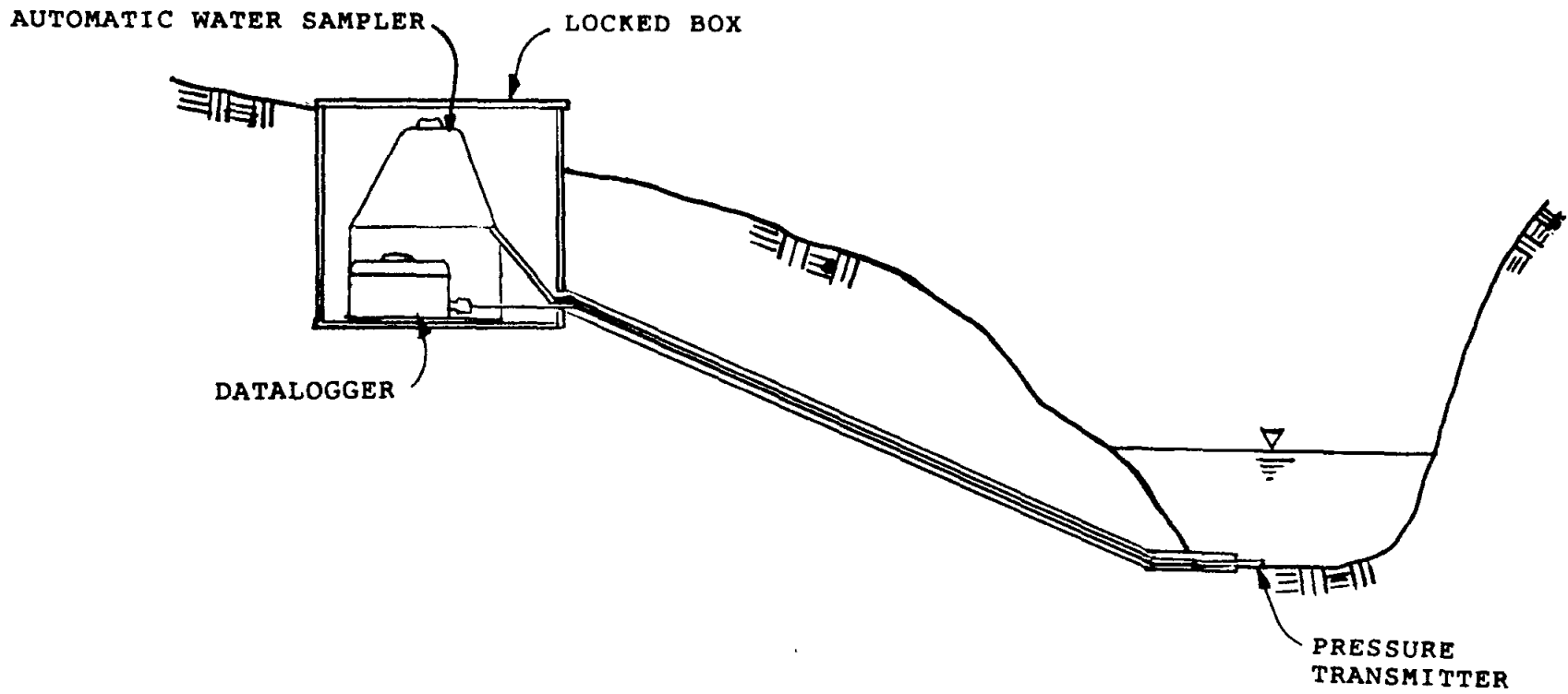
Fig. 2 Typical Water-Discharge and Water-Quality Monitoring Installation
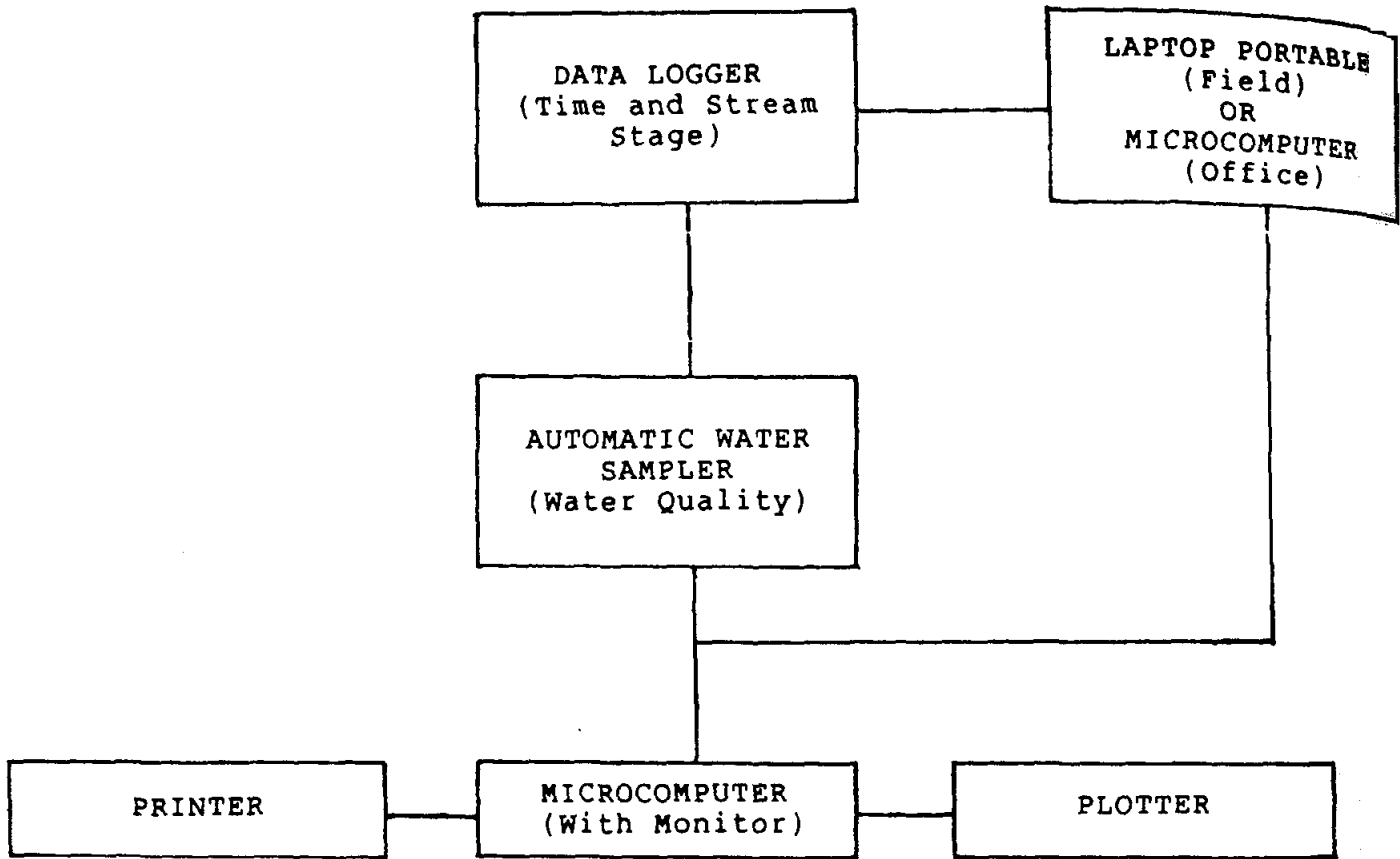
Fig. 3 Primary Hardware Elements for a Computerized Urban Water-Quality
Data Collection System

If several sampling sites and several storm events are sampled each year, the number of samples may approach 100 and may include over 1,000 water-quality data values. Therefore, entering these data into a computer data base may involve major expenditures of personnel time as well as a relatively high probability of data transcription errors. We believe that a better way to transmit laboratory water-quality results for samples is for a laboratory to provide these data on a floppy disk. Many laboratories are willing to supply data in this manner because these data are entered into their computer system or are typed in a report via word processing for transmittal to the client anyway.

Our experience has been that analytical laboratories are able to provide the data in a client specified format. There are many alternative structures that may be used for presentation of water-quality data (Grayman and others, 1988). Two typical structures for water-quality databases commonly available are a value oriented structure and a sample oriented structure. A value oriented water-quality database uses the actual measurement; that is, the laboratory result for a specific water-quality variable as the organizing unit of the database. In the sample oriented water-quality database, the sample itself is the organizing structure and the location and date are not repeated for each water quality variable for which an analysis is performed by the laboratory. Therefore, a sample oriented structure appears to be fairly common for the water-quality databases. However, the type of water-quality database structure should not necessarily govern the format used by the laboratory to transmit the data. Any file structure is acceptable as long as it is usable by both the laboratory and the client.

Table 1 shows a typical data-transmitting file structure for water-quality data. In transmitting the data the laboratory would create such a file for each sample analyzed. The file consists of two parts, header information and water-quality data. The header consists of ten lines containing the location codes, sample date and time, laboratory sample numbers and appropriate remarks. The header information is followed by the water-quality data consisting of 1 line

each for individual water-quality variables analyzed for that sample consisting of two columns on each line. The first column is a sample code and the second column the water quality variable concentration for that sample code. We recommend that USEPA STORET codes be used for sample codes because they are well documented and universally used. The STORET code also could be used as the basis for presentation of tabular data or analysis of water-quality data in the spreadsheet or other software.

Because the water-quality laboratory probably does not have field data collected at the time of sampling, these data are entered into the data file after the data have been received from the analytical laboratory. These data are entered by editing the data file and inserting the appropriate sample code and field water-quality value for a given variable. As additional data are received from the laboratory for subsequent samplings, the data are checked for consistency and appended to a master file containing all the water-quality data for the period of interest.

Computer Software Structure

The water-quality data obtained from the laboratory and edited to include field measurements, including instantaneous discharge at the time the water quality sample was collected, will probably not be in a form readily usable by a typical database system. Therefore, some kind of software may be required to convert the data to a format acceptable to the database, or actually input the data to the database. Although programming languages such as BASIC, FORTRAN, or C can be used to build database management systems, the availability of a multitude of powerful commercial database management systems packages such as DBASE III or :BASE, for microcomputers makes the custom programming approach generally outmoded due to considerations of cost and time of development, documentation and program maintenance. However, selected data calculation routines such as multiple linear regression, hypothesis testing and graphical output may require special computer software.

TABLE 1

Water-Quality Data Transmittal File Structure

Header Information[2]

Field Name	Size	Justify	Field Type[1]	Comments
Project Code	39	Left	Alpha	Project Name Project Number
Station Number	7	Left	Alpha	
Sample Date	6	–	Integer	YYMMDD
Time Sampled	4	–	Integer	HHMM (24 hour clock)
Collector	3	Left	Alpha	Initials
Sample ID	30	Left	Alpha	From sample bottle
Laboratory No.	30	Left	Alpha	
Date Received	6	–	Integer	YYMMDD
Date Reported	6	–	Integer	YYMMDD
Comment	39	Left	Alpha	From Laboratory

Water-Quality Data[3]

Column	Field Name	Field Type[1]	Comments
1	P	Alpha	Letter "P" in Column 1
2 – 6	STORET Code	Integer	
9 – 20	Value	Real	Format: F11.3

Notes: 1) Real data can only contain the following characters:
0, 1, 2, 3, 4, 5, 6, 7, 8, 9, –, +
Integer data can only contain the following characters:
0, 1, 2, 3, 4, 5, 6, 7, 8, 9.
2) The header information should be in the order shown and there should be one line for each field.
3) The water-quality data follow directly after the header information for each sample. It can be in any order and any number or combination of analyses can follow.

Most database management packages have features which permit transporting of the water-quality and streamflow data directly into the database (Weiderhold 1983; Grayman and others, 1988). Some of these features include:

(1) A mechanism for defining the structure for storing data;

(2) Methods for entering data through user defined menus and through transfer from other spreadsheets or data files;

(3) A command language used to control the components of the database including sorting, merging and inquiries of the database;

(4) A programming language that allows for more complex manipulation of the data such as regression analysis;

(5) A report writer for preparing reports based on the data stored in the database;

(6) A graphical display component for preparing graphical output of data stored in the database;

(7) Documentation of the program including manuals, examples and on-line user-friendly menus.

Thus, the most difficult part of using a database management system for analyzing urban runoff water-quality data is getting the data entered into the database. The above elements, including electronic collection of discharge data and laboratory reporting of water-quality data in digital form, are a great aid to entering the data into a urban runoff water-quality data handling system.

CHERRY CREEK BASIN EXAMPLE

Data collected on behalf of the Cherry Creek Basin Water Quality Authority are used as an example to demonstrate the basic time-stage data used to calculate streamflow, water-quality data and load calculations for total phosphorus for an urbanized watershed in the Denver metropolitan area, Colorado.

Streamflow Data

Figure 4 shows a segment of the time-stage data collected in the field by a data logger for the period April 28 to May 1, 1989 for an urbanized watershed gaging station. The elapsed time is in minutes and the value is an arbitrary stage height in feet. A ten minute time increment was used in stream stage recording at this particular station.

Immediately after a storm-event, the time-stage data are retrieved from the data logger using a laptop computer. These data were entered into a FORTRAN program written especially for this multiyear monitoring project which calculates instantaneous stream discharge along with the volume of sample from each sample bottle which should be composited in order to give a flow-weighted composite water-quality sample which subsequently is sent to a commercial laboratory for analysis. An example of the results of the software in converting time-stage data into instantaneous discharge is shown on Fig. 5. The first column of Fig. 5 indicates the elapsed time, the second column the stream stage, the third column the instantaneous discharge and the fourth column the volume of sample at each ten minute increment which must be composited in order to obtain a flow composited sample. Samples by the automatic sampler normally are taken at between 30-minute and 60-minute intervals. Therefore, every third or sixth time point is used to composite the samples taken over the storm hydrograph. The number of water-quality samples by the automatic sampler is usually limited to 24 which is the number of sample bottles in the samples. For most samplers, a maximum of 450 ml is available from each sample bottle, and therefore, the program provides an option for specifying the maximum sample volume from any one bottle of up to 450 ml based upon the maximum instantaneous discharge during the storm.

The same computer program which converts the time-stage data (Fig. 4) into the instantaneous discharge information (Fig. 5) also calculates average daily discharge for a given set of data. Fig. 6 shows an example of average daily discharge calculated from instantaneous discharge for the period April

```
                SE1000B
          Environmental Logger
             05/01   10:45

          Unit# 00000  Test# 0

       INPUT 1:   Level (F)

       Reference          3.65
       Scale factor      10.09
       Offset             0.00

       Step# 0    04/28   12:44

       Elapsed Time      Value
       ------------     ---------
          0.0000         3.65
         10.0000         3.66
         20.0000         3.66
         30.0000         3.66
         40.0000         3.66
         50.0000         3.65
         60.0000         3.65
         70.0000         3.65
         80.0000         3.65
         90.0000         3.65
        100.000          3.65
        110.000          3.65
```

Fig. 4 Example of Time-Stage Data for Streamflow from the Data Logger

SHOP CREEK

STARTING MONTH/DAY/YEAR = 4/28/1989   STARTING TIME = 12:44

REFERENCE =   3.65   SCALE =   10.09   OFFSET =   0.00
STAGE SHIFT =   0.00

ELAPSED TIME (MIN)	STAGE (FT)	DISCHARGE (CFS)	COMP. VOL. (ML)	REAL TIME (HR:MIN)	DATE (MM/DD/YEAR)
0.	3.65	0.47	36.	12:44	4/28/1989
10.	3.66	0.54	41.	12:54	4/28/1989
20.	3.66	0.54	41.	13: 4	4/28/1989
30.	3.66	0.54	41.	13:14	4/28/1989
40.	3.66	0.54	41.	13:24	4/28/1989
50.	3.65	0.47	36.	13:34	4/28/1989
60.	3.65	0.47	36.	13:44	4/28/1989
70.	3.65	0.47	36.	13:54	4/28/1989
80.	3.65	0.47	36.	14: 4	4/28/1989
90.	3.65	0.47	36.	14:14	4/28/1989
100.	3.65	0.47	36.	14:24	4/28/1989
110.	3.65	0.47	36.	14:34	4/28/1989

Fig. 5 Example of Instantaneous Discharge from Time-Stage Data

```
SHOP CREEK STATION SP059.DAT
4/28 - 5/01/89

STARTING MONTH/DAY/YEAR =  4/28/1989      STARTING TIME = 12:44

REFERENCE =      3.65      SCALE =    10.09      OFFSET =      0.00
STAGE SHIFT =    0.04

      AVERAGE DAILY DISCHARGE BASED ON 10 MINUTE INTERVALS

           YEAR      MONTH      DAY      DISCHARGE
                                          (CFS)

           ----      -----      ---      ---------

           1989        4         28        0.89
           1989        4         29        0.53
           1989        4         30        1.02
           1989        5          1        0.28

ENDING MONTH/DAY/YEAR =  5/ 1/1989      ENDING TIME = 10:34
```

Fig. 6 Example of Average Daily Discharge Calculated from Instantaneous
        Discharge

28 to May 1, 1989. Incomplete days, such as the first and last day for this particular time sequence, could be combined with the previous data files to calculate a daily mean discharge for a given day. Daily mean discharge values are stored in a separate daily-values file for use with the water-quality data. Both instantaneous and daily mean discharges are used with the water quality data to provide regression equations and average daily loadings which are discussed in the following sections.

Water-Quality Data

An example of the water-quality data file after editing to include field data is shown on Fig. 7. A typical sample-based file has a ten line header information section for each sample which includes the project name and number, the station ID, the time the sample was collected, the sample ID along with laboratory sample number and the date of sample analysis and reporting. The remaining lines for each sample include the STORET number and the concentration. Field data include water temperature (STORET number P00010) and instantaneous discharge (STORET number P00061). Data for all stations and all samples are included in one large data file. This file serves as input to a FORTRAN program written especially for this project which provides water-quality data reports (Fig. 8), and basic statistics for selected water-quality variables in the data file (Fig. 9).

Additionally, the water-quality data may be manipulated on the computer to perform regression analyses of selected water quality variables. An example of a regression analysis of instantaneous discharge versus total phosphorus concentration is shown on Fig. 10. A FORTRAN program written especially for the project plots the data points and calculates and plots the best fit straight line using cartesian, semilog, or log-log coordinate systems.

Load Calculations in Urban Areas

The water quality data are often coupled with the discharge data to provide load calculations especially for nutrients and heavy metals. Using the same database as illustrated

above, load calculations may be made on either an instantaneous discharge basis or on a daily basis. Fig. 11 shows an example of a daily mean discharge plot for the 1988 water year for an urbanized watershed. Daily mean discharge values are converted to daily total phosphorus load by using the regression plot shown on Fig. 10 for each day. By multiplying the total phosphorus concentrations obtained from Fig. 10 for each mean daily discharge by the mean daily discharge occurring on that day and multiplying that product by a conversion factor gives the daily total phosphorus load in pounds as shown on Fig. 12. Fig. 11 and 12 enable a decision maker to quickly view both discharge and load data to get a picture of the relative importance of flow control on the control of nutrient loadings.

SUMMARY AND CONCLUSIONS

Collecting, analyzing and reporting urban runoff water quality and discharge data requires a specialized computerized data collection and laboratory reporting system. Manually entering stage data and water-quality data into a spreadsheet or other computerized data management system is often prohibitive from both a time and data transcription standpoint. Therefore, discharge data should be collected electronically in the field and water quality data received electronically from the analytical laboratory. Specialized software used to transfer electronic data from data loggers to personal computers are generally available commercially and operate on both laptop and personal computer systems.

Once the data are available on the computer, large numbers of data may be easily manipulated to calculate instantaneous discharge, daily mean discharge, provide water quality basic data reports along with basic statistics for selected water-quality variables, and analyze the data for review by decision makers.

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```
INSITU-Cherry Creek Project 4460
SP
881021
1145

A
88-WI/06052
881022
881111

P00530        10.000
P00610         0.040
P00615         0.020
P00620         6.680
P00625         1.300
P00665         0.120
P00666         0.110
P00671         0.090
P31501        75.000
P31613        65.000
P00672         0.110
P80154         6.000
P90410       308.000
P95440       308.000
P95445         0.000
P95830         0.000
P00010      14.2
P00300       8.2
P00400       8.0
P00095      1100
P99000      3.0
P00061       .69
```

Fig. 7 Example of Water-Quality Data File After Editing to Include Field
Data

WATER-QUALITY DATA

DATE	TIME	TEMPER-ATURE (DEG C)	IN-STAN-TANEOUS STREAM-FLOW (CFS)	SPE-CIFIC CON-DUC-TANCE FIELD (US/CM)	SPE-CIFIC CON-DUC-TANCE LAB (US/CM)	OXYGEN, DIS-SOLVED (MG/L)	PH FIELD (STAND-ARD UNITS)	PH LAB (STAND-ARD UNITS)	SOLIDS, RESIDUE AT 105 DEG. C, SUS-PENDED (MG/L)	NITRO-GEN TOTAL (MG/L AS N)	NITRO-GEN AMMONIA TOTAL (MG/L AS N)	NITRO-GEN NITRITE TOTAL (MG/L AS N)	NITRO-GEN NITRATE TOTAL (MG/L AS N)
10/15/87	1500.	—	19.00	—	398.	—	—	6.8	104.	7.31	1.36	0.28	2.73
10/28/87	1115.	—	0.54	858.	1190.	—	8.1	8.0	6.	9.80	-0.02	0.02	9.28
11/16/87	1430.	—	4.80	—	154.	—	—	7.4	32.	2.46	0.22	0.05	1.51
11/23/87	1145.	12.5	0.69	1100.	1180.	10.6	—	8.2	6.	9.20	-0.02	0.02	8.68
12/21/87	1210.	8.0	0.69	1780.	1130.	14.6	8.4	7.9	158.	10.50	-0.02	0.01	9.09
01/15/88	1520.	8.0	1.20	2820.	—	7.6	7.9	—	32.	6.00	0.30	0.08	4.92
01/25/88	1040.	7.0	0.69	1400.	—	10.9	8.1	—	-2.	10.00	-0.02	0.01	9.09
01/28/88	1235.	7.0	4.40	852.	—	9.1	7.4	—	172.	3.80	1.02	0.05	1.15
02/12/88	1455.	8.5	5.60	423.	—	9.4	7.3	—	60.	2.89	0.34	0.03	0.96
04/03/88	1250.	15.0	2.60	800.	—	8.4	8.2	—	26.	4.98	0.14	0.08	4.10
04/12/88	1240.	16.5	0.74	850.	—	7.1	8.2	—	4.	10.80	0.07	0.05	9.05

Fig. 8   Example of Water-Quality Data Report

VARIABLE	N	MEAN	STD. DEV.	MINIMUM	MAXIMUM
TEMPERATURE (DEG. C)	9	11.6	5.0	7.0	22.0
INSTANTANEOUS STREAMFLOW (CFS)	25	12.87	12.46	0.29	45.00
SPECIFIC CONDUCTANCE, FIELD (US/CM)	23	642.	667.	115.	2820.
SPECIFIC CONDUCTANCE, LAB (US/CM)	5	810.	444.	154.	1190.
OXYGEN, DISSOLVED (MG/L)	9	9.4	2.3	7.0	14.6
PH, FIELD (STANDARD UNITS)	22	7.6	0.4	7.0	8.4
PH, LAB (STANDARD UNITS)	5	7.7	0.5	6.8	8.2
SOLIDS, RESIDUE AT 105 DEG. C, SUSPENDED (MG/L)	25	122.	191.	-2.	696.
NITROGEN, TOTAL (MG/L AS N)	25	5.18	3.45	1.29	13.02
NITROGEN, AMMONIA TOTAL (MG/L AS N)	25	0.35	0.42	-0.02	1.71
NITROGEN, NITRITE TOTAL (MG/L AS N)	25	0.09	0.11	-0.01	0.40
NITROGEN, NITRATE TOTAL (MG/L AS N)	25	3.05	3.36	-0.02	9.28
NITROGEN, TOTAL KJELDAHL (MG/L AS N)	25	2.04	2.41	0.50	13.00
PHOSPHORUS, TOTAL (MG/L AS P)	25	0.404	0.286	0.040	1.030
PHOSPHORUS, DISSOLVED (MG/L AS P)	25	0.229	0.170	0.030	0.810
PHOSPHORUS, ORTHO, DISSOLVED (MG/L AS P)	25	0.167	0.136	-0.010	0.660
PHOSPHORUS, ORTHO, TOTAL (MG/L AS P)	25	0.211	0.154	-0.010	0.690
CARBON, ORGANIC TOTAL (MG/L AS C)	5	17.	8.	6.	32.
TOTAL COLIFORM, MFIMENDO (COLS/100 ML)	13	9847.	26179.	-1.	99999.
FECAL COLIFORM, 24-HR MEM. FIL. (COLS/100 ML)	22	8170.	20941.	-5.	99999.
BOD OXYGEN DEMAND, BIOCHEM. CARBON 5-DAY (MG/L)	5	5.	3.	-1.	10.
SUSPENDED SEDIMENT (MG/L)	4	64.	51.	11.	146.
ALKALINITY, LAB (MG/L AS CACO3)	21	108.	108.	6.	338.
BICARBONATE, LAB (MG/L AS HCO3)	21	132.	132.	7.	412.
CARBONATE, LAB (MG/L AS CO3)	21	0.	0.	0.	0.
HYDROXIDE, LAB (MG/L AS OH)	21	0.	0.	0.	0.

(1) MINUS SIGN MEANS "LESS THEN" INDICATED VALUE.   (2) —— MEANS NO DATA AVAILABLE FOR SAMPLE.

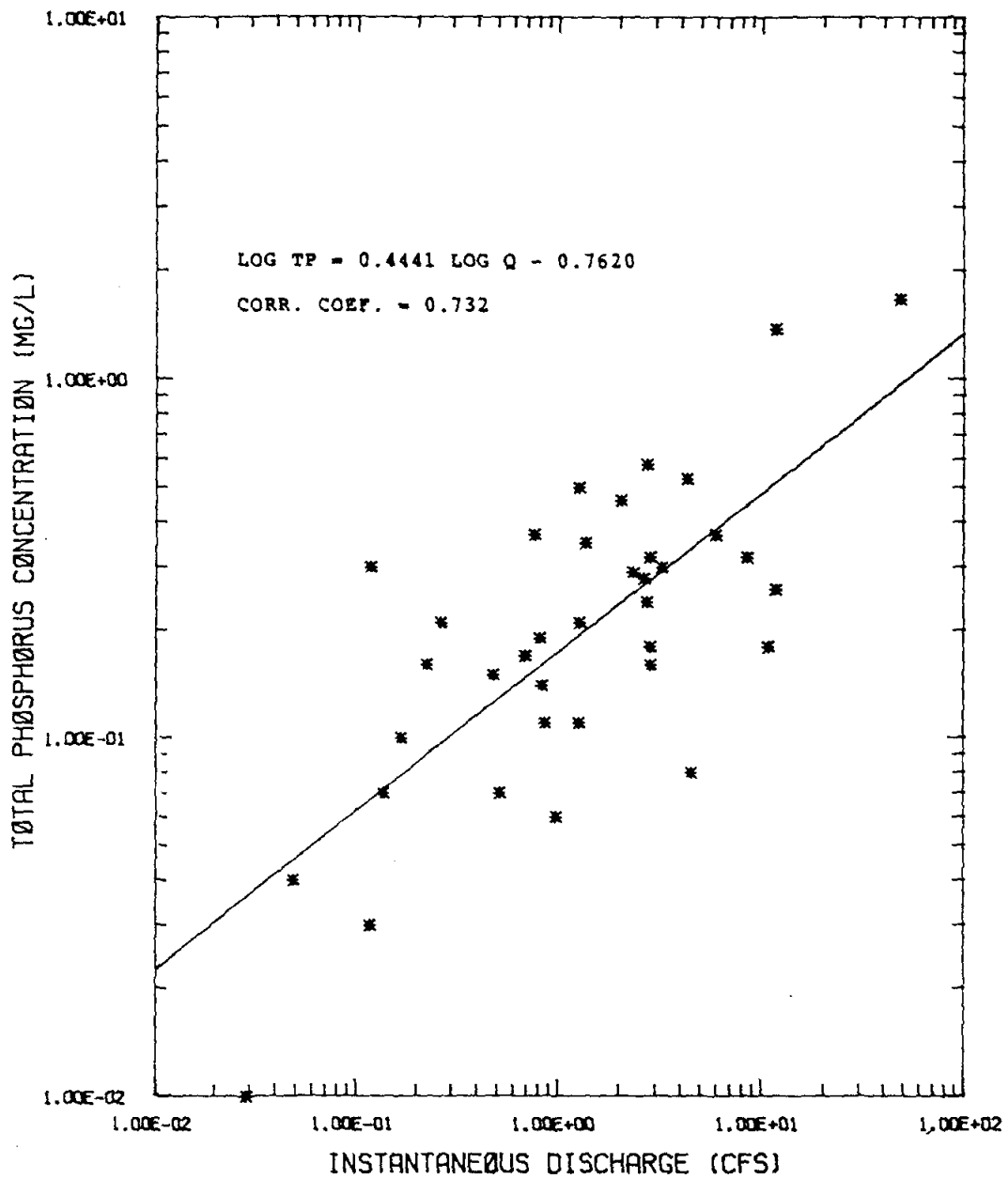Fig. 9 Example of Water-Quality Basic Statistics Report

Fig. 10 Example of Regression Analysis Plot of Instantaneous Discharge vs.
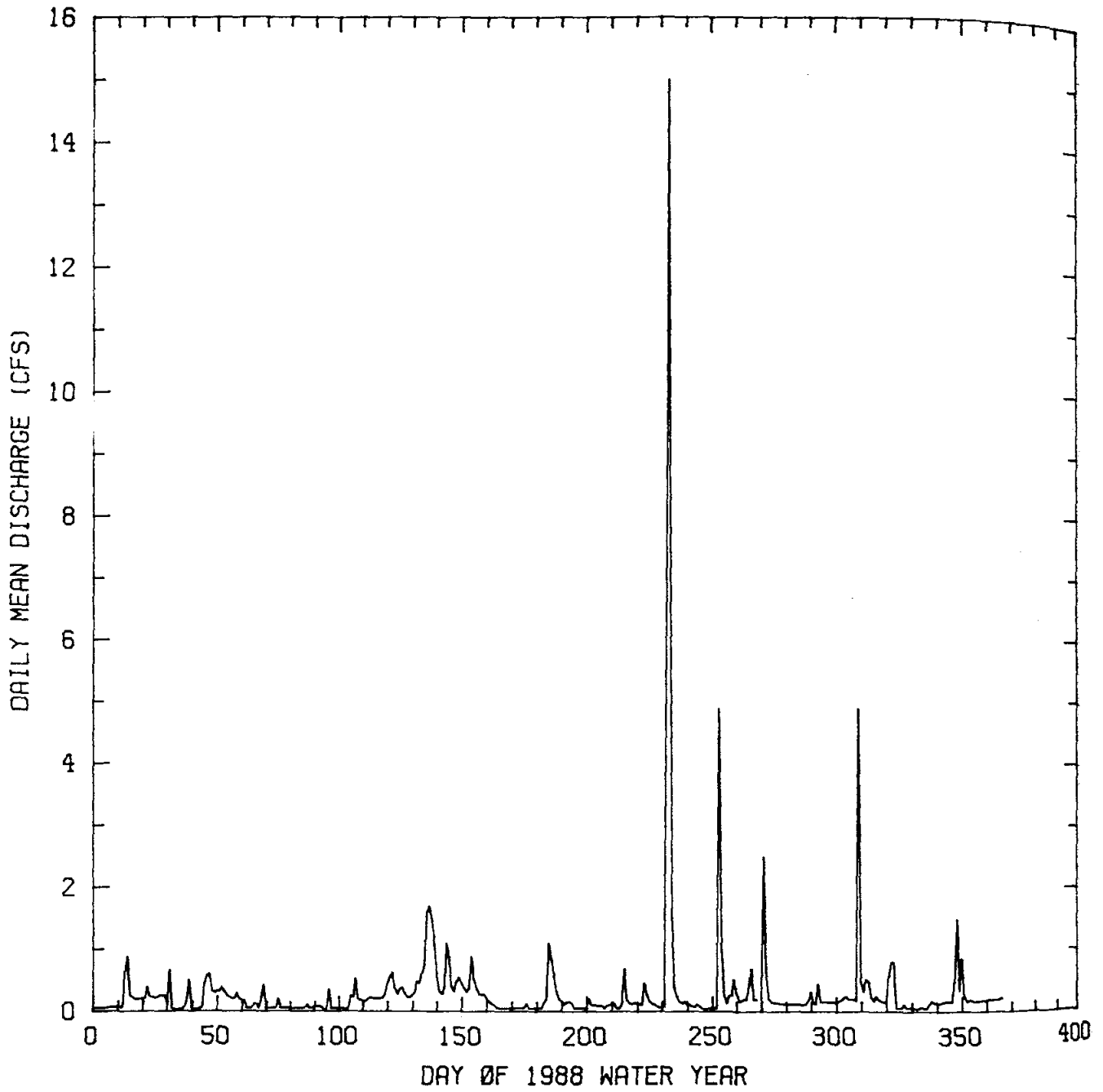Total Phosphorus Concentration

Fig. 11 Example of a Daily Mean Discharge Plot for the 1988 Water Year
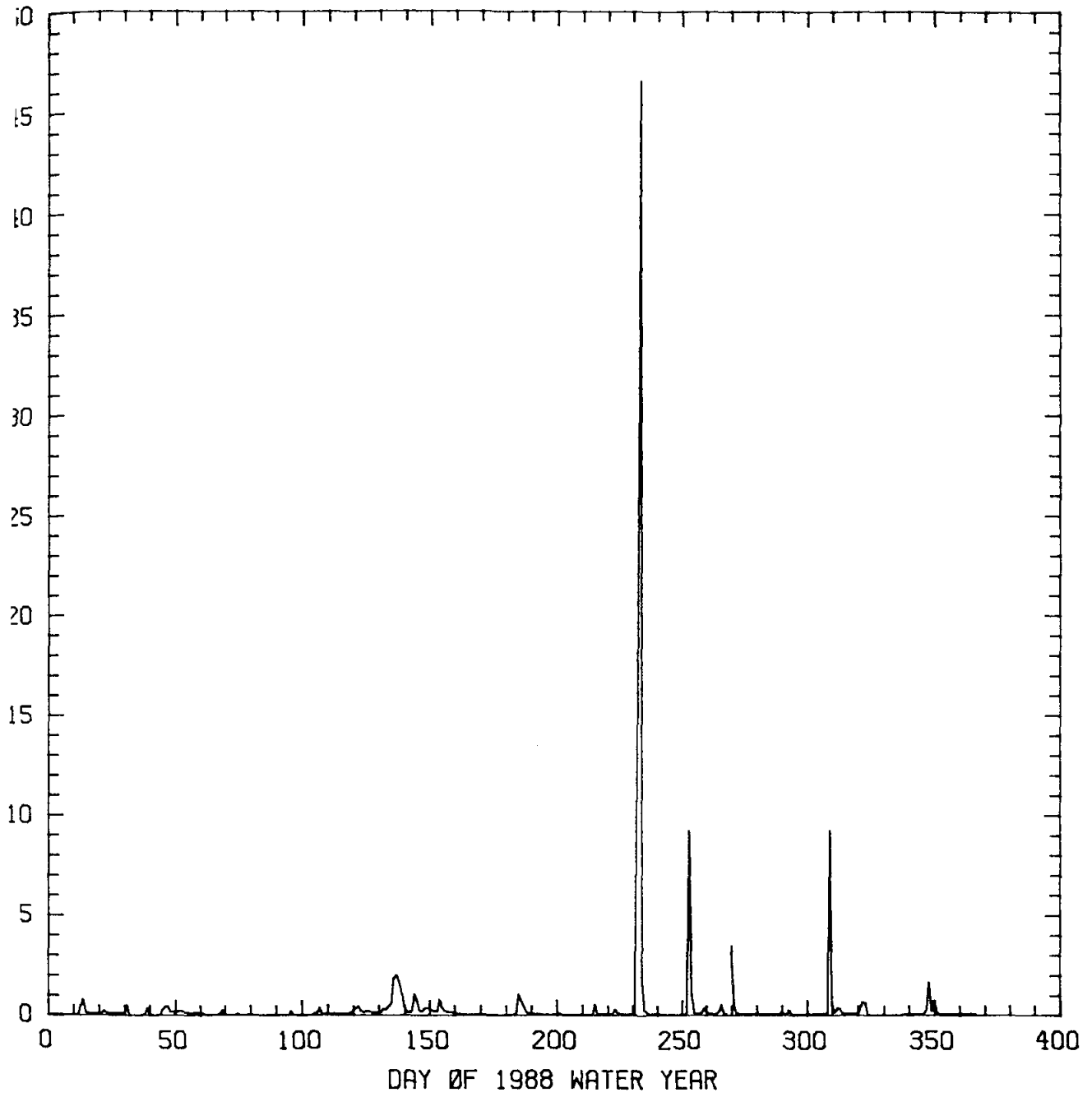
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Fig. 12   Example of a Daily Total Load Plot for the 1988 Water Year

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Banquet Address

International Symposium on the Design of Water Quality Information Systems
Banquet Address

BIOLOGICAL MONITORING OF WATER QUALITY

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ABSTRACT

Biological monitoring is carried out to confirm that previously established water quality conditions important to the indigenous biota are being met. No instrument devised by humans can measure toxicity or integrate in a biologically meaningful way the aggregate impact of all stresses to which the indigenous biota is exposed. It is, of course, a sine qua non that, without chemical/physical monitoring data, the factors that produced the biological response will either be unknown or less well quantified than they should be. Therefore, biological monitoring is meant to be carried out as an important component of a biological/chemical/physical water quality monitoring system. Biological monitoring can provide early warning information on material from municipal or industrial wastes about to enter an aquatic ecosystem. This would prevent damage by blocking waste entry or by using information about the condition of the biota in the aquatic ecosystem itself to indicate the onset of a trend that, if allowed to continue, would result in serious harm. Both early warning and in-system monitoring units can be designed so that they are compatible with computer information systems, and the time of information generation is markedly reduced. Some of these early warning systems that are suitable for computer interfacing are described along with management options that become available with the utilization of computer interfaced biological monitoring systems.

JUSTIFICATION FOR THE EXTENSIVE USE OF BIOLOGICAL MONITORING OF WATER QUALITY

In the early stages of the Industrial Revolution, both industrial and municipal discharges into aquatic ecosystems were generally small in volume, with relatively little toxicity, and widely spaced. In the relatively few cases when severe damage occurred, the aquatic ecosystem, particularly a river, often had the opportunity to recover some distance downstream. Nonpoint source discharges did not contain persistent pesticides nor were they heavily enriched with artificial fertilizers. However, both the magnitude of the insults and their frequency, including spacing, have greatly increased since that time. In short, the unmanaged natural system is incapable of assimulating societal wastes, and the services and amenities provided by the aquatic ecosystem are in considerable jeopardy. Not only have local impacts become more intense, but danger is evident from a new source, regional or global impacts on aquatic ecosystems from such events as acid rain and/or global warming. For effective management, biological responses due to local anthropogenic wastes and stresses must be separated from those arising from afar or having a global impact.

The situation is not without parallel. The Agricultural Revolution, which was in a sense a great leap forward in environmental management, resulted from the fact that the

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unmanaged environment was not producing food in either the quality or quantity that human society felt it deserved. While some inequities are still present in this regard, there is no question that, without managing the environment in the way that resulted in the Agricultural Revolution, the earth could not support its present population, let alone that projected for the year 2000 and beyond. The unmanaged environment is clearly incapable of coping with all of the insults generated today, and the effects are present globally in increased amounts of carbon as carbon dioxide in the atmosphere, in acid rain, and in the deterioration of aquatic ecosystems in this country and elsewhere. Some remarkable restorative efforts can be cited, such as the Thames River and Lake Washington in the United States, but, in the absence of a mangement system designed to maintain established water quality conditions, their rehabilitation is likely to be short lived.

The Agricultural Revolution that led to widespread environmental management to produce food was not without its costs to human society. Similarly, the environmental management revolution will not be without its costs either. Nevertheless, the cost of the absence of management has been all too evident in the recent Alaskan oil spill and the global loss of species. The Alaskan oil spill furnishes an excellent example of the value of preventative measures. The ecosystem's services (for more details see Ehrlich and Mooney, 1983) to the tourist industry as a commercial and recreational fishery have been lost for an indefinite period. The cleanup, which almost certainly will only be partially effective, and the subsequent efforts to recolonize damaged areas may never get the ecosystem back to its predisturbance condition. Even if this is accomplished, 10 or 20 years will undoubtedly be needed before full ecological condition is achieved. Ecosystem services can no longer be reliably maintained with an unmanaged system or a system in which the resource management is fragmented. Only integrated resource management, including biological monitoring, has a chance of keeping ecosystems in suitable condition for long-term sustainable use that provides all desired amenities and services.

THE RELATIONSHIP BETWEEN BIOLOGICAL MONITORING AND CHEMICAL/PHYSICAL MONITORING

Determining the concentration of a potential toxicant in an aquatic ecosystem without accompanying biological information may lead to poor management decisions because necessary information is lacking. The chemical information alone may be misleading because: (1) some chemicals may be toxic on a long-term basis at levels below present analytical capabilities; (2) water quality strongly mediates the toxic response; and (3) other chemicals may act synergistically (or antagonistically) with the chemical in question, markedly altering the toxic response.

Ruth Patrick (personal communication) has found that certain forms of chromium may be concentrated by diatoms over 70,000 fold, their concentration in the ambient water. In this case, the analysis of the water column alone might provide grossly misleading information as to the concentrations to which the indigenous organisms are exposed. Additionally, time is a major factor in determining the toxic response, and merely knowing the concentration of the chemical to be safe for acute exposure does not inevitably lead to the conclusion that it is safe for long-term exposure. Even if the response under long-term exposure conditions is known, it may well not be known for a particular range of environmental quality necessary for making an informed judgment for a particular aquatic ecosystem.

It has been known for years (e.g., Water Quality Criteria, 1972) that water hardness, pH, temperature, and other characteristics markedly influence the toxic response to heavy metals and a variety of other chemical substances. If the response under each particular water quality were known, a much better projection could be made than if only one response under one water quality is known. However, generally, even for the most common toxicants, the information base in this regard is inadequate. An estimated 76,000 chemicals are in fairly common use and many millions are on the American Chemical Society Computer

Registry of Chemicals (e.g., Maugh, 1978). These numbers, coupled with the fact that there are relatively few toxicologists, make it highly improbable that an appropriate array of information will be available to make an accurate prediction of response given a particular set of water quality conditions. The most prudent way to determine this is by actual biological testing, which is often less expensive than sophisticated chemical analyses.

Synergistic interactions (the toxicity of the combined chemicals is more than their individual additive toxicities) have been well known for years. In some cases, particular kinds of synergistic interactions have been published (e.g., Doudoroff and Katz, 1953). In other cases, the synergistic interaction may not have been previously known. Years ago when I was teaching and carrying out research during summers at the University of Michigan Biological Station, a kill occurred with the lamprocide TFM that was not predicted from the exposure conditions. After being informed of the incident, I carried out a few tests with the material and zinc and found that, under certain water quality conditions, a probable synergistic interaction had taken place. The point is that well defined mixtures of chemicals are rarely tested under laboratory conditions, and, even when they are, synergistic interactions are not always evaluated in the necessary detail to generate a usable perdictive model.

Presence of colloidal materials in the water may affect the toxicity of heavy metals and other chemical substances in a variety of ways. Additionally, temperature is a well-known modifier of toxicity. The simplest way of analyzing such a complex set of chemical/physical variables with regard to the toxic response is to test this response directly with living material.

EXTRAPOLATION OF BIOLOGICAL MONITORING RESPONSES

Since the purpose of biological monitoring is to ensure that previously established water quality conditions are being met (surveillance would be the word used if measurements were taken in a systematic and orderly fashion without mandatory corrective measures when certain thresholds have been exceeded) and is intended to protect natural systems, a key organism or a key character or quality of the ecosystem could be selected and used to predict the responses of all other components. For example, a persistent belief has been that if the most sensitive species could be selected and protected it, all other species associated with it would be inevitably protected (e.g., Weis, 1985). This reasoning has some serious flaws (e.g., Cairns, 1986), the most notable one being that a species sensitive to substance A may be quite tolerant to substance B, while another species may have just the reverse situation. After searching through literally thousands of chemicals, one was found (TFM) to which the sea lamprey infesting the Great Lakes appeared to be most sensitive, at least among the fishes. Every chemical presumably has a most sensitive species, but no single species is most sensitive to all chemicals or even 70 or 80% of them (e.g., Mayer and Ellersieck, 1986). One of the chief U.S. Environmental Protection Agency's most prominent research toxicologists (Mount, 1987) urges that the search for the most sensitive species be stopped and attention given to other more important matters.

The key question, of course, is one of information redundancy. In short, how much information can be reliably predicted from a particular piece of information without additional tests? Unfortunately, only a few tests on aquatic biota and ecosystems deal with information redundancy. One of the early papers on this subject (Kaesler et al., 1974) shows a respectable amount of information redundancy for some groups with regard to other groups. The types of information chosen for that analysis suggest diatoms would be the best overall group, although aquatic insect larvae showed some information redundancies that could not have been easily predicted. If biological monitoring is to be used extensively in a cost-effective way as a primary monitoring technique, such redundancy analyses should become more common in the selection of qualities, or characteristics of choice might be greatly reduced for particular aquatic ecosystems.

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Pratt and Cairns (1985) showed that functional groups of protozoans had a remarkably consistent pattern and relationships despite vast differences in the component species making up these groups. In short, while the species might not always be the same, the activities appear to be. When a species representing a particular functional group disappeared, another one with the same general functional capabilities appears to take its place.

Some of the evidence in the preceding paragraph, particularly Pratt and Cairns (1985), shows that aquatic invertebrates, in this case protozoans, at the species level may appear chaotic with some species being present at one sampling location, others being present at another. A pattern, however, emerges when the species are grouped according to their function rather than by their taxonomic designation. This, of course, merely reflects the often repeated observation that, as one proceeds upward in the heirarchy of biological organization from subcellular to cell to tissue to whole organism to population to community and to ecosystem, new properties emerge at each level of biological organization that could not be discerned at lower levels. This leads to several inescapable conclusions that have been widely ignored in many biological monitoring efforts: (1) that neither structural nor functional attributes at higher levels of biological organization can be inferred from data collected at lower levels, and (2) that what appear to be dramatic changes at lower levels of biological organization may not necessarily produce comparable changes at higher levels of biological organization. This is not to say that information at any level of biological organization is inappropriate or misleading, but rather that reliable extrapolation from responses at lower levels of biological organization to those of higher levels of biological organization does not seem to be reliable with the present information base available. Therefore, all monitoring programs should include information at higher levels of biological organization as well as appropriate lower levels until some of these problems are sorted out.

Many of the measurements made for purposes of biological monitoring could be inelegantly categorized as "critter counting." This type of structural information (e.g., community structure, trophic relationships, saprobien ratings, etc.) is very useful and has formed the core of biological assessment of pollution in aquatic ecosystems for many years. However, functional attributes, such as detritus processing, nutrient spiralling, and the like, are also extremely important and, with some notable exceptions (e.g., Bormann and Likens, 1979 or Likens et al., 1977), have not had the prominence that they should have. Cairns and Pratt (1986) have commented on the relationship between structural and functional analyses of ecosystems and point out three possible relationships between structural and functional parameters in aquatic communities:

1. The two parameters are so intimately linked that one cannot change without changing the other; therefore, measuring either structure or function will predict what is happening in the other.

2. Many species have similar functions. This collectively ensures considerable functional redundancy for most of the major attributes of aquatic communities. As a consequence, the loss of a species is possible without a significant reduction in species richness. Since function is more conservative than species richness, the latter is the more sensitive measurement.

3. Species can be stressed sufficiently to alter their functional capacity without eliminating them from the aquatic community. If so, functional capacity might be significantly impaired without the array of species being altered, at least in the short term. Thus, functional measurements would provide an earlier warning of major changes in the aquatic community than would structural measurements.

What should be measured, then? Estimates of functional responses (e.g., primary productivity, detritus processing)

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ignore the processing organisms, may be highly variable, and may have little meaning to the general public. Most conservation groups fail to get fired up about altered rates of detrital processing, and newspapers with pictures of dead fish and banner headlines are more likely to catch the public's attention. Critter counting ("not as many mayflies below the plant discharge") wins the public relations battle. What the public fails to realize, however, is that most of the mass and energy flow in ecosystems passes through the unseen organisms, the microbial processors. These are not the most popular toxicity testing species and are not always included in field studies of larger organisms.

Given the state of statistical procedures and the power and speed of most large computers, it is no longer reasonable for "critter counters" to equivocate when confronted with questions of environmental impact. The organisms will integrate the effects. Huge species lists can be statistically reduced and the array of water quality measures combined. Factors linked to community structure can be identified, and the vast amount of information in species lists can be used to compare sites and systems. If ecosystems were simply constructs of processing elements that do basically the same tasks, Hutchinson's question, "Why are there so many kinds of animals?" would have long ago been answered. With the present state of knowledge about the relationship between structure and function, both types of measurements should be carried out in any biological monitoring program until one determines whether extrapolations from one to the other are reliable.

An illustrative example of the questions to be asked when determining structural and functional attributes in a biological monitoring program follows.

Structural attributes

1. Are the numbers and kinds of species of all major groups of organisms typical of a balanced biological community present?

2. Is the data base on diversity, rarefaction, and other indices sufficient to distinguish normal variability from long-term trends?

3. Are all age classes of organisms with long life cycles present, and are all species reproducing at a rate sufficient to maintain viable populations?

4. Are normal food webs or food chains present and functioning?

Functional attributes

1. Is primary production being carried out at a normal rate (that of a balanced biological community) by the indigenous species?

2. Are the bio-geochemical processes characteristic of this specific type of ecosystem proceeding at characteristic rates?

3. Are the nutrient spiralling and energy transfer processes occurring in ways characteristic of this particular ecosystem?

4. Are the colonization rates adequate to support normal successional processes?

TYPES OF MONITORING TO BE PERFORMED

Types of monitoring to be performed, frequency of the monitoring, level of detail, and geographic area to be covered should all be highly correlated with the decision being made. Although it is a sine qua non that ecologists must play a strong role in making these decisions, their efforts will be less effective if the use of the information in the decision making process is not carefully considered. Decision analysis is commonly used in a number of other professions and even in the field of ecology. However, many ecologists are not even aware of the literature on decision analysis, and an even smaller number have actually used the process. My discussion here assumes three major goals for

biological monitoring: (1) to maintain balanced biological communities, (2) to protect both the structural and functional integrity of ecosystems, and (3) to protect biodiversity.

The term "balanced biological community" almost certainly would be defined differently by a randomly chosen assortment of ecologists. "Balance" could be defined in terms of the proportion of organisms at each trophic level, in terms of species dominance, or in terms of the successional process that would incorporate such things as the MacArthur-Wilson equilibrium model (MacArthur and Wilson, 1963). The second goal, protecting structural and functional integrity of ecosystems, could be defined in terms of bio-geochemical cycling or in a variety of other ways. Goal three, protecting biodiversity, has recently been given considerable scientific and public attention that has resulted in such meetings as the National Forum on BioDiversity (co-sponsored by the U.S. National Academy of Sciences and the Smithsonian Institution; Wilson, 1988) or the Symposium on Biotic Impoverishment (sponsored by the Woods Hole Research Institution; Woodwell, in press). Extinction of species is occurring at a rate far in excess of previous centuries, and possibly at a rate unprecedented on earth. If too many species are lost (and no one knows how many constitutes too many in ecological terms), maintaining the other community qualities mentioned will be difficult.

Periodic Collection of Data from Permanent Plots or Sites

The periodicity of data collections will depend on the statistical need to distinguish normal cyclic variation (or even ordinary variation within natural limits) from a trend. Unfortunately, trend analysis has not been investigated indepth for most ecological systems. This is particularly true for freshwater aquatic systems. In fact, despite abundant chemical/physical data, Smith et al. (1987) have indicated that it is impossible, based on present evidence, to establish reliable trends for chemical/physical water quality.

Criteria for Selection of Sites for Extensive Surveys

Criteria for selecting sites, frequency of sampling, and level of detail required (together with a number of other factors) should all be determined by considering the ways in which the information will be used to make management decisions. Management is used in this connection with regard to water quality control in the sense that corrective or preventive action will be taken when necessary to ensure that natural systems stay within predetermined quality control parameters.

The second major criterion for site selection is determining the extent of variability of natural systems so that normal cyclic variation is not confused with a trend. This means that the sites would have to be sampled not only extensively but over a long period of time. Presumably, if the information redundancy investigations are carried out carefully, a significant reduction in the amount of effort necessary will result.

A third major criterion for carrying out extensive surveys is to enable decision makers to make a distinction between regional, pollutional, and other stresses and global stresses. This distinction will not be an easy one because the effects will most likely be a series of gradients extending from local and easily identifiable effects to long-range effects where multiple sources are contributing to degradation.

Criteria for Selection of Sites for Intensive Monitoring

Again, I am making the assumption that the purpose of monitoring is to provide an early warning system to signal when the system has gone beyond certain predetermined quality conditions or that the ecosystem is staying within these conditions as predicted. Intensive monitoring could serve as an error control feedback loop to show that predictions of safety were unfounded or that some unexpected event has caused excursion beyond predetermined values. In this case, the speed of information generation should be the major determinant (e.g., Cairns et al.,

1970). Therefore, the parameters selected for measurement, whether chemical, physical, or biological, should ideally be amenable to direct computer interfacing. For example, the respiratory rhythm of fishes has been amenable to such direct interfacing. The ORSANCO system has a number of chemical/physical parameters already being measured with the utilization of a direct computer interfacing network. The parameters being monitored should be key characteristics (similar to body temperature, heart rate, and blood pressure for human condition monitoring). If these parameters are outside normal boundaries, they have a high probability for indicating serious consequences in other parts of the system. Once a computer interfaced system is set up, the frequency of sampling is almost irrelevent because the cost incurred is minute for additional information. The system is running all the time, and the important aspect is to avoid an information overload. This can be done with a microprocessor that ensures that information is gathered at appropriate intervals. A number of statistical techniques are available that analyze such information, even if it is in cycles on a diurnal or some other basis. The location of these early warning system probes is exceedingly important, and no easy method is available to ensure that no major informational gaps occur. Freshwater systems should always have probes above and below the confluence of major tributaries with a river system, in addition to above and below major industrial sites, etc. In some cases, extensive sampling of a river or lake can be carried out on a one time only basis to determine which portions provide information similar to other portions; a reduced number of sites can be selected on this basis. There is also the possibility of establishing some sites with continual or nearly continual monitoring with computer interfaced systems. Other sites may have extensive sampling on a periodic basis. The ORSANCO system uses both approaches in combination, resulting in considerable effectiveness for chemical/physical parameters only. Useful material on statistical considerations associated with determining sites for intensive surveys and intensive monitoring can be found in Green (1979) and Pielou (1977).

SELECTION OF MONITORING/SAMPLING PARAMETERS

Biological, physical, and chemical parameters should be selected for their predictive value. This predictive value might be divided in two categories. The most important category is the instant recognition of striking changes in key parameters that indicate major deleterious ecological effects. The second is being able to distinguish between normal variability and the onset of a new trend. Unfortunately, little direct scientifically justifiable evidence is available to indicate the predictive value of the most commonly used parameters.

FUTURE NEEDS

In the introduction to this volume, Robert C. Ward pointed out that Naisbitt, in his 1982 book entitled Megatrends, describes how our society is evolving into an information society and points out that "uncontrolled and unorganized information is no longer a resource in an information society. Instead it becomes the information of the information worker ...... information technology brings order ..... and therefore gives value to data that would otherwise be useless." I have used biological monitoring in a pro-active sense; that is, it is information designed to provoke immediate action when the system being managed signals that something has gone out of control. I deplore the use of biological monitoring as a mere data gathering activity, which unfortunately is the common usage. Even the term "surveillance" seems too strong if no action is intended, but, at least, it is more accurate. Biological monitoring has developed an enormous methodology base but as Macek (1982) notes, the amount of data generated by environmental toxicologists is overwhelming. He is also correct in stating that our knowledge has not greatly increased as a consequence of this expansion of the data base. More data are needed, of course - they always are! However, our biggest failing is not using effectively the data we have in an ecosystem quality management program. This is particularly true of water ecosystems where appropriate ways of integrating information have been evident for

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years, but regulatory measures are so prescriptive that only problems are perceived in a fragmented fashion rather than in a holistic fashion. Ecologists have generally failed to describe explicitly the qualities of an aquatic or other ecosystem that must be maintained to preserve biological integrity. Only then can an effective pro-active management program be developed. As we attempt to develop an appropriate information system, we will undoubtedly find that we have focused entirely too much on single species toxicity tests and not enough on other types of information appropriate to protecting the integrity of aquatic ecosystems. Until we determine the qualities to be protected and the means to monitor the system so that we have a feedback loop telling us when the system is out of control, we will not have an effective management program. Biological monitoring is just another form of data gathering unless it is used as an integral part of an ecological quality control system. It is in the use of the data, not the collection of data, that has been our greatest failure to date!

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Data Analysis

THE BULL RUN WATERSHED AS A WATER QUALITY INFORMATION SYSTEM

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ABSTRACT

The Bull Run watershed provides drinking water to approximately 700,000 people in the Portland, Oregon metropolitan area and is the only municipal supply watershed in the United States with legislatively mandated raw water quality standards.   The goals of monitoring in the Bull Run watershed are to assure continued production of high quality potable water and to provide information describing the physical processes operating within the watershed.   Monitoring, a cooperative venture involving the USDA Forest Service, the City of Portland, and the USDI Geological Survey, is used to determine compliance with the water quality standards at five locations within the watershed and to assess effects of individual projects on local site water quality. The monitoring network, consisting of 19 fixed stations and 14 temporary stations, produces over 15,000 individual analyses annually.   The water quality standards are based on nonparametric time series analysis, paired basin regression relationships and allowable exceedance ratios. Data are routinely computerized and statistically analyzed using a combination of personal computer applications.   Interpretations of temporal and spatial water quality data are presented in technical compliance reports.   Water quality information is also used to modify existing project activities as necessary.   (KEY WORDS: water quality, monitoring, nonparametric statistics, Bull Run watershed.)

Introduction

The Bull Run watershed provides drinking water to approximately 700,000 people in the Portland, Oregon metropolitan area. This 67,000 acre (165,490 hectares) watershed is located approximately 30 miles (18.6 kilometers) east of Portland and two miles (1.2 kilometers) south of the Columbia River. The watershed is closed to public access.

Public Law 95-200 was established in 1977 and allows management activities which maintain the historic levels of high water quality. The Forest Service has a conservative harvest/salvage program which abides by Public Law 95-200. The goals of monitoring in the Bull Run are to assure continued production of high quality potable water and to provide information leading to a better understanding of the physical processes operating within the watershed.

Standards

The law requires the Forest Service, in cooperation with the City of Portland, to develop raw water quality standards. The Bull Run watershed is the only municipal supply watershed in the United States with legislatively mandated raw water quality standards.

The Bull run water quality standards are based on six statistical tests: time series (Figure 1), paired basin regression, acceptable exceedance ratio, test for shift, mean with tolerance limits, and detection limits (USDA Forest Service, 1984). The primary test is the nonparametric time series analysis of 15 physical, chemical and biological variables. Time series intervals vary for each of the variables depending on available historical data. Most of the periods are 14 days long.

Paired basin regression analysis is also used as a method of comparing current and

historic data. One of the subbasins, Fir Creek (Figure 2), has not had any road construction or timber management with the exception of one small 14 acre clearcut on the top of a ridge near the headwaters. This subbasin is used as the control subbasin for comparison with other locations in the watershed. Paired basin regressions based on historic data were established between the Fir Creek subbasin and the other four subbasins. Significant paired basin regressions are established for flow, temperature, conductivity, turbidity, suspended sediment, nitrate, tannin and lignin, and total organic carbon.

The acceptable exceedance ratio test was developed to compare data between the control subbasin and the other three stream stations when a paired basin regression was not valid.

Trends are investigated using the Paired T-test of the period means. Quarterly, bi-annual and yearly trends can be estimated.

Twenty-three other variables are analyzed on a yearly basis. Tolerance limits and analytic detection limits are used to identify changes in these variables. These variables are metals, pesticides and other chemical constituents such as alkalinity and sodium.

Monitoring

The Bull Run monitoring network (Figure 3) is used to determine compliance with the raw water quality standards at the five required stations and to assess effects of individual projects on local site water quality (USDA Forest Service, 1987). The monitoring is a cooperative venture involving the USDA Forest Service, the City of Portland, Oregon and the USDI Geological Survey. The network consists of three different types of stations, Key, Source Search, and Project stations.

The standards apply to the five Key stations. Four of the Key stations are located at the base of the four major subbasins and one is located below the reservoir system at the intake to the distribution system (Headworks). Sampling frequency for each variable is specified in the standards and is

based on historical sampling frequency. Generally, weekly visits are necessary at the stream key stations and daily samples are taken at the Headworks.

Source Search stations supplement the compliance monitoring by providing upstream information within each subbasin. The data are used in determining the general condition of the watershed, to measure the response of the watershed to natural and man-caused effects, and to track the effects of management activities downstream. Most of these stations are located just above stream confluences and are sampled weekly.

Project stations are used to evaluate the water quality effects of an activity. Most of these stations are located directly above and below the project activity. In some cases, suitable "above" sites are not available and paired basin stations are used.

Whenever possible, pre-activity data is collected so that project effects can be estimated during and after the project. Sometimes, emergency conditions occur that preclude adequate sample collection before an activity begins. Post activity monitoring usually includes a complete storm season after activity completion.

Project stations are sampled frequently during activities, 1-3 times per week, and less frequently before and after the activity. The variables to be monitored at a project are determined by the type, extent, and location of the project. Turbidity, suspended sediment, and fecal coliform are usually sampled at all projects. Intensive monitoring at project stations is done on a relative short term basis depending on the specific activities.

Water quality monitoring at the Project stations is used in conjunction with Procedural and Inventory monitoring.

Procedural monitoring assures contract specifications are accomplished and water quality protection measures are implemented correctly. Examples of this monitoring are checking that oil absorbent pads are placed under certain equipment and that streamside management units are properly located.
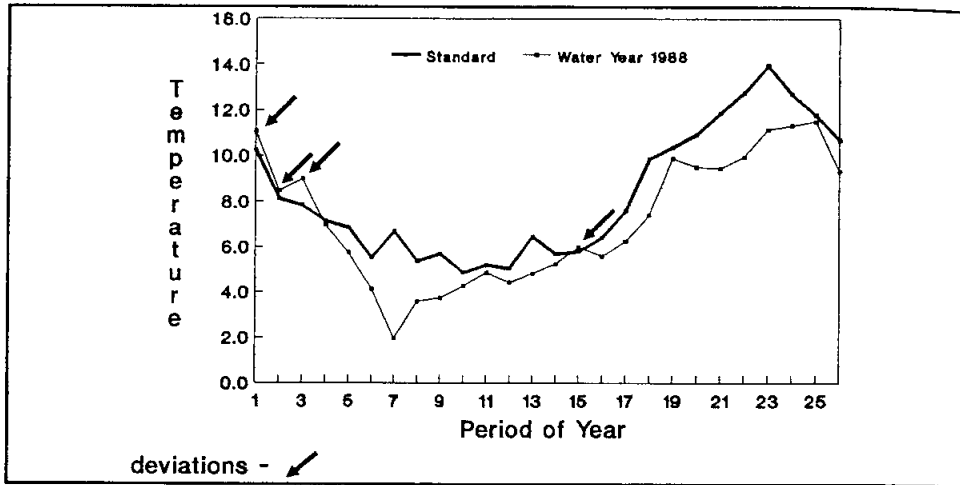
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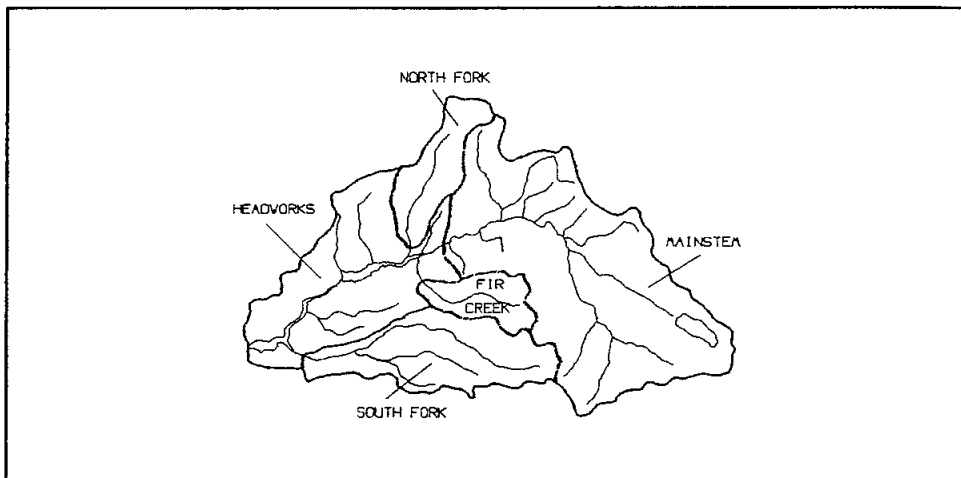**Figure 1** – Example Time Series Standard for Temperature at Fir Creek

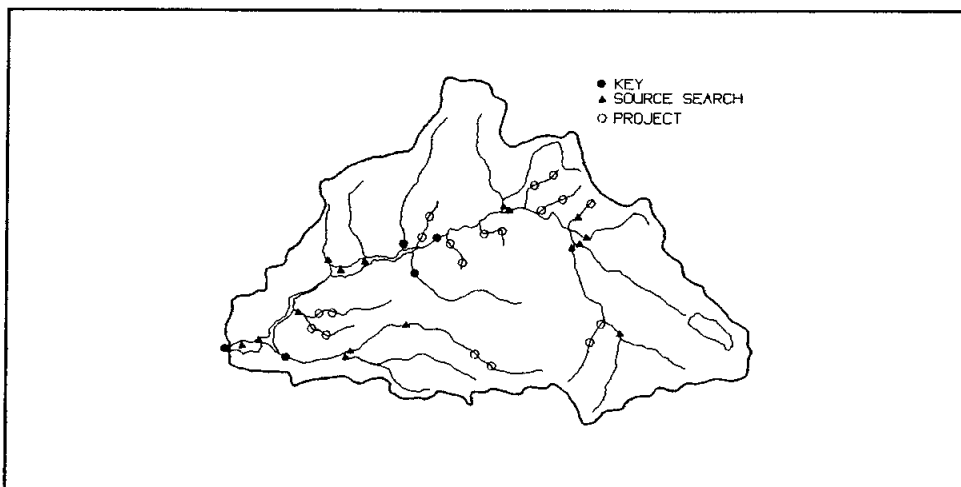**Figure 2**-Subbasins within the Bull Run Watershed, Oregon

Figure 3 – Monitoring Stations in the Bull Run Watershed, Oregon

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Inventory monitoring estimates changes in the physical environment that are not determined with water quality analysis. At present, this involves measuring stream shade and debris movement before and after a project.

Storm sampling is initiated when flows increase above defined thresholds at each stream Key station. At present, these thresholds represent about a one or two year storm event. The storm samples are collected at all the stations and analyzed for turbidity, suspended sediment and total phosphorus.

All of these monitoring processes are used to determine whether 'best management practices' on the projects are sufficient to protect water quality. Information from this monitoring can be used to adjust operating procedures, and to separate natural effects from forest management effects.

Reporting

Immediate detection of extremely abnormal water quality is accomplished by the water quality analysts at the City of Portland Water Quality Lab. Criteria for abnormal data are specified in the standards. If an abnormal water quality condition is detected, the standards require an immediate search for the source of the abnormality with both water quality monitoring and field reconnaissance.

Current data are compared to the standards and deviations determined after the water quality data have been reviewed for errors and electronically transferred to the Forest Service. Presently there is a lag of three to five days between the completion of the sample analysis and the reporting of deviations.

Bi-weekly reports are prepared that attempt to explain any deviations from the standards. These reports use available hydrologic data, knowledge of environmental processes, and information about all management activities within the watershed to assess the cause of the deviation.

Most of the deviations have been considered due to a natural process, due to

the operation or maintenance of water storage or hydropower activities, or are unexplainable. Some of the unexplainable deviations are the result of overly sensitive standards which were developed from data which historically had been reported with more significant figures than are reliable.

Information from the standards compliance process, along with procedural monitoring data, is used to detect any changes in the water quality of the Bull Run as quickly as possible. Ongoing management activities can be revised or halted if they are determined to be adversely affecting water quality. Monitoring information is quickly analyzed so that any natural, adverse event can be recognized as soon as possible.

Interpretive reports are also prepared for each management project which is monitored. These reports assess any on-site activity impact and, using the Source Search stations, evaluate the transport of any on-site impacts downstream within the subbasin.

Nonparametric statistics are used in the data analysis to analyze the changes in the differences between the stations rather than documenting the changes at each of the stations. Since watershed conditions normally change over time (the basis for the time series standards applied at the Key stations), comparing pre, during and post activity periods can mislead conclusions made concerning the effects of a project. Therefore, comparison of similar periods during each year monitored is used along with comparisons of pre, during and post periods.

Information from the project reports is used for several purposes. After completion of a project, the effectiveness of the Forest Service's Best Management Practices can be assessed for the protection of water quality. On-site effects of the management activities can be defined and the downstream transport of any on-site effects can be estimated. With this information, future management activities can be planned with some knowledge of the potential for, and magnitude of, on-site and downstream effects of certain management activities and appropriate mitigation measures.

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Revisions

Monitoring of Bull Run water quality has been an evolutionary process. With increased knowledge of the environmental processes, advancement in technologies of water sampling and chemical analysis, refinements in statistical data analysis, and improvements in technology transfer, the monitoring program continues to be progressive.

Recently, a Task Force of three water quality experts reviewed the Bull Run monitoring plan and concluded that the Bull Run produced exceptionally good quality water with little room for improvement (Aumen, Grizzard and Hawkins, 1989). They reported an absence of any detectable deterioration in the present water quality from historical levels.

They recommended the following improvements for the monitoring program:

With the new, automated sample collection instrumentation and advances in electronic mechanisms for data transfer, recommendations were made for sampling frequencies to be dependent on flows and for continuous instream measurements to be made when possible. Access to real time data would give the quickest response to any abnormal water quality. The City of Portland is already in the process of getting continuous instream measurements for turbidity, pH, conductivity and temperature with the ability to change sampling frequencies depending on stage.

Connected with the previous recommendation was the suggestion for revising the standards and incorporating flow weighted analysis for the variables which are strongly correlated with flow.

Increased sampling at the reservoirs to define the processes which occur there was recommended. Since the reservoirs are a collection basin for the stream inputs, small undetectable changes in the water quality of the streams could be accumulated in the reservoirs and become detectable or change the natural processes within the reservoirs.

A shift to increased emphasis on procedural monitoring with less emphasis on the water quality monitoring at the Source Search stations was recommended. The Forest Service has now documented the Procedural monitoring requirements and implementation steps so that information can be conveyed formally. The recommendation for the reduction and/or elimination of source search station monitoring has been met with skepticism and a decision concerning this recommendation will be made during the planning for implementation of the Task Force recommendations.

A change in the goals of the project monitoring was recommended. Presently the goals are to assess the water quality effects of the project activities at several sites for a limited time period based on the potential risk to water quality. The risk is estimated from such factors as proximity to streams and reservoirs or stability of the site. The Task Force recommended choosing a few sites, conducting long term research monitoring, and intensifying the possible impacts of the project. The purpose of the research would be to gain a better understanding of the natural processes and responses to disturbances.

The three experts estimated that dissolved solids from rainfall contributed approximately 60% of the dissolved solids in the streams. A warning was made that without documentation of atmospheric inputs, changes in the atmospheric inputs of both precipitation and dry fall could result in change in the water quality which could then be falsely attributed to management activities. Therefore, they recommended sampling the atmospheric sources at several locations within the watershed.

The last recommendation was to conduct 'freeform' analysis on the data already available to gain information of natural processes within the watershed.

Conclusions

The information system created through monitoring of the Bull Run watershed provides knowledge of the present condition of the water quality and quantity, provides an increased awareness of the processes which

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occur within the watershed, and determines if water quality protection measures used at different project activities are adequate for the protection of the water quality. Through the cooperation of the three agencies, land and water management activities are accomplished and water quality data effectively becomes information. This information is used for planning future activities in the watershed as well as being the basis for changing the way operations are conducted.

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A GROUNDWATER MONITORING PROGRAM FOR THE SANTA CRUZ RIVER PIMA COUNTY, ARIZONA

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ABSTRACT

A groundwater quality monitoring program was established along the effluent-dominated reach of the Santa Cruz River to investigate potential impacts of recharged secondary treated effluent. A database-management system was developed to assist in data reduction and analysis. Database design focused on providing users with the required applications through a menu-driven interface. The developed system plays an integral part in the dynamic decision-making process. Data from the monitoring program are presented to demonstrate the procedures used for data analysis during the initial sample rounds. General mineral characteristics between monitor wells, background wells and discharged effluent are compared using Stiff diagrams and simple trend analysis. Results from trace constituent monitoring are presented. Procedures are discussed to refine future monitoring emphasis based on the current results.

INTRODUCTION

Pima County is located in the Sonoran desert of southeastern Arizona and contains the Tucson metropolitan area. County-wide population is approaching 680,000. By the year 2005 an estimated one million people will live in the county. The county is completely dependent on groundwater for its domestic and industrial water supplies.

Pima County Wastewater Management Department (PCWWMD) manages county wastewater collection and treatment, operating two treatment plants and 11 smaller outlying facilities. The two major plants have dis-charged treated effluent to the Santa Cruz River since the early 1970s. Currently, 50 million gallons per day (mgd) of secondary effluent is discharged to the river. The Santa Cruz is an ephemeral stream that has natural flow only during major storms. An estimated 80 percent of the discharged effluent is recharged to groundwater.

The two major facilities operate under National Pollutant Discharge Elimination System (NPDES) permits. Process control parameters and traditional pollutants, such as biological oxygen demand and suspended solids, are monitored along with a wide array of trace inorganic and organic constituents. Reissued NPDES permits have steadily increased the number of monitored and regulated trace inorganic and organic constituents. Quarterly or monthly influent and effluent wastewater data for many important trace constituents are available from mid-1985 to present. The sampling strategy for wastewater monitoring is imposed by NPDES permits, although special sampling projects have been performed to obtain baseline data on constituents of interest not regulated in the permits.

Arizona is implementing stringent aquifer protection regulations based on the recently enacted Environmental Quality Act of 1986. To determine the potential affects of wastewater recharged along the Santa Cruz, PCWWMD established a groundwater-monitoring program along the effluent-dominated reach of the river in 1988. This program will be the main emphasis of this paper. Other PCWWMD groundwater monitoring programs include outlying facilities using recharge basins/evaporation ponds and county-owned landfills.

The monitoring programs described above were developed independently to monitor and protect Pima County's groundwater resource. Ideally, these programs would have been designed to be compatible with each other, because they are inherently related. However, federal and state environmental regulatory activities are increasing rapidly. These activities often are not integrated, which creates difficulties when developing new monitoring programs. Another complicating factor occurs when the county develops programs to investigate environmental concerns not addressed by other agencies, such as the monitoring program along the Santa Cruz. The problems PCWWMD face concerning groundwater monitoring programs are to identify whether effluent discharge adversely affects groundwater quality along the Santa Cruz and if the current monitoring program is adequate. One step toward solving these problems was the development of a computerized water quality information management system to reduce, analyze and integrate data from various monitoring programs to support the decision-making process.

The purpose of this paper is to present the procedures used by PCWWMD to manage and analyze water-quality information from the groundwater monitoring program along the effluent-dominated reach of the Santa Cruz River. A brief description of the sampling plan will be presented, followed by a summary of the database structure and design. Data from the current program will then be presented in order to investigate data analysis techniques and future monitoring objectives.

SAMPLING PLAN

Development of the sampling strategy for the groundwater monitoring program along the Santa Cruz was a complex process. The major goal of the program was to investigate possible trace-constituent pollution of groundwater from recharged effluent. The number of possible pollutants to monitor was extensive, so primary and secondary drinking water constituents, along with the priority pollutants were emphasized. Another

important goal of the project was the development of a long-term monitoring strategy.

Much inorganic groundwater quality data exists for the area adjacent to the effluent-dominated reach of the Santa Cruz (Wilson et. al. 1984). Most of this data has been obtained from irrigation or domestic water wells that were not designed for monitoring groundwater quality. This data can be useful for obtaining historical and background constituent levels. However, suitable wells for sampling the groundwater immediately below and adjacent to the river were lacking.

During the first half of 1988, 12 monitor wells were installed (Figure 1). Depth-to-groundwater ranged from 80 to 300 feet. Currently, samples are collected quarterly. A quarterly sampling frequency was chosen to explore possible seasonal differences in constituent concentrations.

Wells are analyzed for general minerals, nitrogen species, trace metals and purgeable halocarbons and aromatics (EPA Methods 601 and 602). During the first year, one sample at each well will be analyzed for the remainder of the priority pollutants not analyzed for in the above tests. Currently, three samples from each well have been obtained.

DATABASE MANAGEMENT SYSTEM

Hardware and Software Configuration

The initial step in database design was to examine current computer capabilities. The department was equipped with IBM PC/XT- and AT-compatible microcomputers with a minimum of 640K RAM and 20-megabyte internal hard disks. The department was committed to dBase III Plus as their PC-based data-management software. To enhance system flexibility, modems were installed to allow input and output to other computers. Removable 20-megabyte disk units were added to ease data transfer and backup. A dBase compiler, Clipper, was purchased to increase application performance and to allow compiled programs to be executed on other machines without the dBase III Plus software.
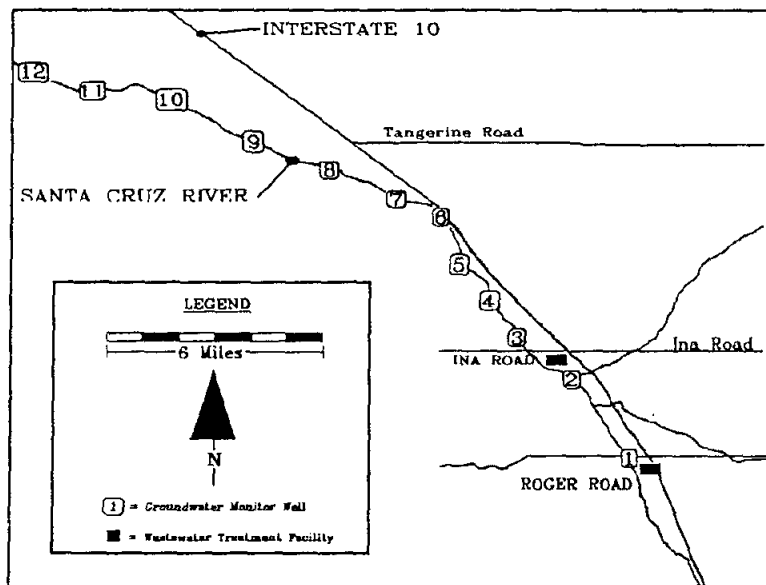
Figure 1. Groundwater Monitor Wells Along Santa Cruz River near Tucson, Arizona.
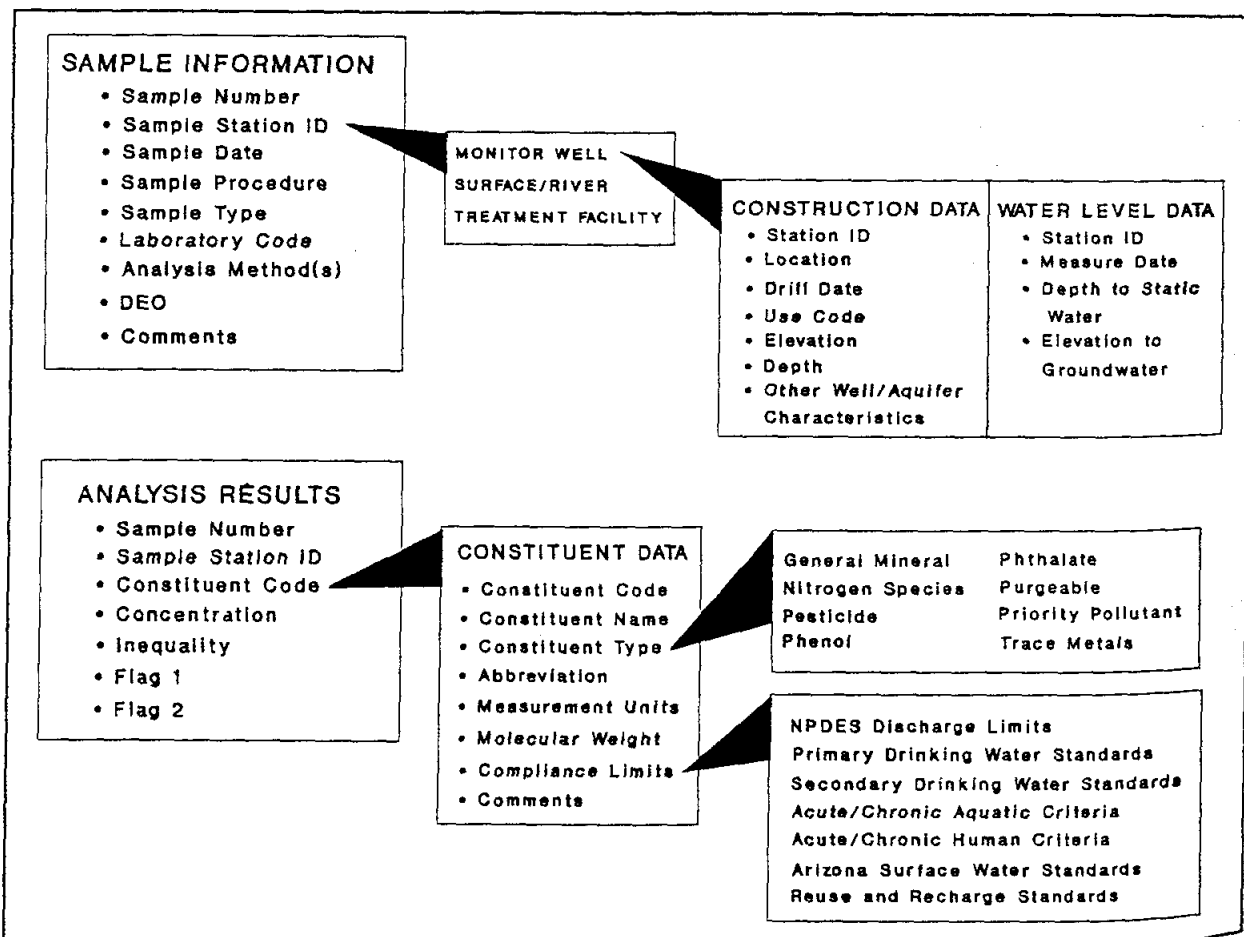

Figure 2. Summary of Database File-Structure.

Database File-Structure

Database file-structure is dependent on the type and amount of data expected. Data from the wastewater monitoring program was examined to define important information. Because water quality data is generally similar, overall file structure design could remain constant for various monitoring programs. Large amounts of data were anticipated, so one goal of file-structure design was to reduce the number of files and fields per record to minimize processing time and storage requirements.

The database was designed around two main data files that contained sample information and analysis results (Figure 2). By exploiting the relational capabilities of the database software, fields per file were minimized by using certain fields within files as relational keys to link multiple data files. Sample number and station identification are the keys used to store, retrieve and link analysis results. A sample station can be a monitor well, a surface or river sample site or a treatment facility. For monitor wells, construction and water level data are linked using sample station identification.

The analysis results file is the one that is most often manipulated to retrieve information, so efficiency of structure is important. The inequality field marks results that are less than the laboratory reporting limit with a "less than" sign. The reporting limit is entered for the concentration. The two flag fields are used to annotate individual results. The first flag contains a code indicating any problem with the analysis or if the sample was a blank or spike. The second flag marks when a particular result should not be used in calculations because of severe problems with the analysis. The description of each flag code is located in a separate file.

Information about each constituent is stored separately and related to the results file by constituent code. The main purposes of the constituent file, other than storing constituent name and abbreviation, are to keep track of compliance standards and to provide a means to select groups of constituents for analysis. Current and proposed water-quality limits are maintained in this file, along with dates of promulgation and reference documents. Analysis results can then be filtered to report results greater than current or anticipated future standards.

In order to enhance data interpretation capabilities, groups of constituents often need to be examined or manipulated. A field was added to the constituent data file to facilitate this process. This field contains abbreviations of selected groups the constituent belongs to. For example, mercury has the entry "TM" for trace metal and "PP" for priority pollutant. When a user picks a group of constituents for analysis, this field is tested first during processing to determine if a constituent should be disregarded, or selected for further manipulation based on previous menu selections.

Database Design

The database design primarily focused on identifying required or useful applications and then enclosing the developed applications in an easily operated user interface. The goal was to develop a menu-driven system that allowed the user easy access to data without having to learn the database software. This would concentrate the users effort on interpretation of the data rather than on learning techniques to manipulate the data. Anticipated users were consulted during initial application definition and throughout application development to ensure appropriateness and consistency.

The most important function of the menu-drive was to provide a means for users to view and print raw or summarized data in several formats. The system developed allows the user to select any combination of sample stations and constituents for examination. Common groups of constituents, like the primary drinking water constituents, can be selected as a group, versus individual selection. When sample stations and constituents have been selected, the user can filter the data in various ways including: detected results only, results exceeding current or proposed regulatory standards, or results greater than a user-defined value.

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Two report formats were designed that present results by individual well for groups of constituents, or by a single constituent for a group of wells. At this point in the monitoring program, examining simple trends over sample rounds is an effective form of analysis. Reports are generated in chronological order. When a user requires a report format not available as a menu option, a generic report format can be downloaded to word-processing software for user specific enhancements.

Graphical representation of the data is also a valuable technique for providing trend analysis. The user enters the graphics subroutine of the database system and selects well, constituent and result filters as described above. A data file is then created that is compatible with a separate graphics software package. The user temporarily leaves the database menu to prepare the required plots. Macros and/or templates have been created to assist the user when preparing commonly used plots. Typically, several constituent concentrations are plotted versus time in a line-graph format to detect changes over time.

A descriptive statistical summary of the data also can be generated, corresponding to the two types of report formats described above. Included in the summary are the number of analyses, number of samples above reporting limits, arithmetic mean of detected values, median value of all results and maximum value.

MONITORING RESULTS AND DISCUSSION

The most difficult aspect of the monitoring program was determining the best methods for data analysis. During initial sampling, limited data would be available to support decisions concerning groundwater quality and the direction and intensity of future monitoring. Statistical analysis of groundwater data is desirable, but until a sufficient number of sample results are available, statistical analysis is premature. During the interim, however, results still must be analyzed for decision-making purposes.

General Minerals

An initial objective was to investigate whether the monitor wells were sampling

recharged effluent. Stiff diagrams (Hem 1985) were used to compare general mineral water quality characteristics. These diagrams were selected because they are easy to generate and provide a visual representation of the data.

Groundwater samples from an upgradient well and a well adjacent to the Santa Cruz that are not likely effected by recharged effluent were compared with samples from the monitor wells and the river using Stiff diagrams (Figure 3). The general mineral water quality of the monitor wells is closer to that of effluent-dominated Santa Cruz than to the selected background wells. Groundwater quality of the area adjacent to the Santa Cruz channel is complex (Wilson et. al. 1984), and more background well data is needed to fully characterize the indigenous water quality. In order to provide more information to characterize the groundwater sampled by the monitor wells, bromide concentrations will be obtained. The chloride/bromide ratio can then be used to assist in groundwater characterization (Koglin 1984).

Nitrate and chloride concentrations in groundwater recharged by secondary treated sewage effluent is of major interest to PCWWMD. Nitrate was the most variable constituent in the first three samples rounds. A complex pattern of nitrate concentrations among wells was discovered, versus a relatively constant concentrations of other minerals, including chloride (Table 1). Wells SC-10, 11 and 12 approach the primary drinking water standard of 45 milligrams per liter (mg/l) as nitrate. Wells SC-04 and SC-06 also show elevated nitrate concentrations. There also seems to be a general trend of increasing nitrate concentration from wells SC-08 through 12. Perhaps even more interesting are the low nitrate levels in wells SC-01 and SC-07. Some differences between sample rounds are present, indicating possible seasonal differences.

Chloride often is used as an indicator constituent when investigating the effects of sewage effluent on groundwater quality. Chloride concentrations are relatively constant between wells, except for SC-11, which is considerably lower. Comparison between sample rounds are seemingly consistent,
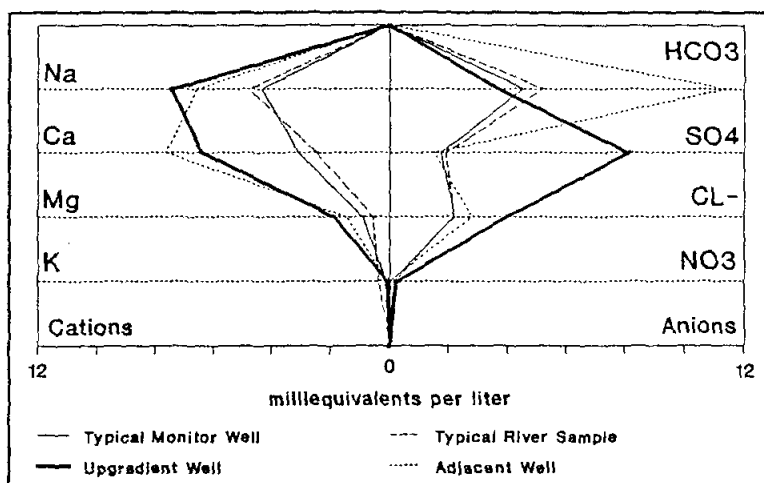
Figure 3. Comparison of Stiff Diagrams.

Table 1. Nitrate (as NO_3) and Chloride Concentrations (mg/l) for the Santa Cruz Monitor Wells.

Well	Summer 1988		Fall 1988		Winter 1989	
	Nitrate	Chloride	Nitrate	Chloride	Nitrate	Chloride
SC-01	1.3	80.0	0.9	79.6	2.2	76.1
SC-02	26.6	69.7	27.9	76.5	29.2	86.4
SC-03	10.2	80.4	20.4	82.8	20.4	88.8
SC-04	33.2	75.0	37.7	83.9	28.4	72.9
SC-05	22.2	72.6	20.8	70.4	21.3	74.7
SC-06	22.6	55.9	33.4	59.5	18.2	63.0
SC-07	2.2	76.5	1.8	80.7	3.1	78.2
SC-08	15.1	83.2	13.7	85.0	10.2	81.1
SC-09	19.0	55.9	19.5	57.4	19.5	59.8
SC-10	36.8	65.5	44.3	62.3	44.3	62.0
SC-11	39.0	36.5	42.1	38.9	42.1	36.5
SC-12	35.0	70.2	40.3	70.1	37.7	64.2

indicating no conspicuous seasonal differences. Chloride concentrations do not vary proportionally with changes in nitrate concentrations.

Without substantially more data, statistical analysis of the data is not feasible. In the interim, a number of objectives for long-range monitoring have been identified. First, quarterly monitoring for general minerals will continue. The additional data should allow a statistical determination of seasonal differences in nitrate and other constituent concentrations. The additional data also will allow differences between wells to be determined more accurately. The goal is to possibly relax monitoring frequencies for statistically similar wells or constituents in order to concentrate resources on wells or constituents of more interest.

One area of concern is the source of nitrate in the high nitrate wells. State regulations may soon require effluent denitrification prior to recharge. Little data is available concerning whether effluent causes significant increases in nitrate levels in groundwater of Santa Cruz basin or if sewage effluent is the sole cause of the high nitrate levels. The monitor wells with the highest concentrations of nitrate (SC-10, 11 and 12) are also the wells closest to extensive agricultural activities. At wells with high nitrate levels, nitrogen isotope analyses will be initiated. Analysis of these results should help identify the source of nitrates.

Trace Constituents

The primary objective of the monitoring program was an investigation of possible trace constituent contamination of groundwater from recharged effluent. Table 2 presents effluent trace constituent data for both treatment plants from April 1985 through December 1988. This data shows that trace inorganic and organic contaminates are frequently discharged to the Santa Cruz, occasionally at concentrations exceeding current primary drinking water standards.

Monitoring for trace inorganic constituents in the groundwater has shown only a few detected compounds. Arsenic, barium and lead were detected at or near their reporting limits at several wells. However, all detected results were well below the primary drinking water standards.

Monitoring for trace organic constituents in the groundwater, with the exception of one analysis, has shown no detected priority pollutants. At monitor well SC-03, chloroform was detected at 0.6 micrograms per liter ($\mu g/l$) in the first sample after well construction. Subsequent sampling has shown no detectable chloroform, and the initial result was attributed to chlorinated drinking water added to the borehole during the drilling process.

The results from the first three sample rounds indicate that recharged secondary treated effluent is not causing trace contaminate pollution of groundwater along the Santa Cruz at detectable levels. The results are not yet conclusive, so monitoring will continue. However, monitoring frequency may be reduced to once per year based on the current results. If trace contaminants are detected, monitoring frequency can again be intensified.

Statistical Analysis

Statistical analysis of data was considered from the outset of project development. Many problems surface when trying to perform statistical analysis of groundwater monitoring data. First, the underlying assumptions about the sample population necessary for typical statistical analysis (i.e. independent, normally distributed, random variables) may be violated. Second, when constituents are reported at less than detection limits, typical statistical analyses are again questionable because any estimated value used in calculations will be biased in some way (Gilliom and Helsel 1986). Finally, current compliance regulations are based on single numerical values as a violation of standards, rather than as a method that accounts for measurement and analytical variability.

These factors and others influence the approach taken toward statistical analysis of this groundwater monitoring data. The development of the monitoring program was

TABLE 2.   Summary of Trace Constituents in Secondary Effluent Discharge to
the Santa Cruz River.[1]

CONSTITUENT	NUMBER[2] ANALYZED	PERCENT DETECTED	MEDIAN[3]	MEAN[4]	MAXIMUM	MCL[5]
TRACE INORGANICS						
Arsenic	206	49	4.0	5.7	29.0	50.0
Cadmium	219	81	0.9	3.6	190.0	10.0
Chromium	204	79	< 5.0	6.0	48.0	50.0
Lead	206	80	4.6	7.6	50.0	50.0
Mercury	209	47	< 0.2	0.8	2.6	2.0
Silver	206	80	2.0	3.4	80.0	50.0
TRACE ORGANICS						
4-chloro-3-methylphenol	120	13	< 1.0	6.7	33.2	
2,4-dichlorophenol	125	10	< 1.0	6.3	27.7	
2,4-dimethylphenol	123	10	< 1.0	4.5	18.0	
2,4-dinitrophenol	100	10	<13.0	12.9	19.5	
phenol	129	19	< 1.0	7.9	60.0	
2,4,6-trichlorophenol	126	13	< 1.0	6.3	24.0	
bis(2ethylhexyl)phthalate	39	51	3.8	50.3	773.0	
butylbenzyl phthalate	40	25	< 1.0	11.5	28.1	
diethyl phthalate	36	36	17.0	33.7	104.0	
di-n-butyl phthalate	38	37	2.5	7.5	17.8	
1,2-dichlorobenzene	181	14	< 1.0	2.2	6.4	
1,4-dichlorobenzene	182	20	< 1.0	1.5	3.0	75.0
toluene	49	16	< 1.0	3.1	6.0	
chloroform	174	83	2.5	3.4	14.0	
methylene chloride	168	45	< 1.0	2.9	15.5	
tetrachloroethene	171	18	< 1.0	12.5	62.4	
1,1,1-trichloroethane	168	11	< 1.0	1.6	2.8	2000.0

[1] Constituents analyzed consistently at undetected levels in effluent not
shown.
[2] Samples from April 1985 to December 1988. All concentrations in ug/l.
[3] Median based on all sample results.
[4] Mean is average of detected values.
[5] EPA Primary or Secondary Drinking Water Standards (ug/l).

considered a dynamic process: the initial sample rounds were expected to help identify the statistical approach to take toward future sample rounds. When enough samples are available, the methods described by Harris et. al. (1987) will be used to characterize the groundwater quality of the general mineral constituents, including nitrate and chloride. The constituents will be tested for seasonality, normality and serial dependence. Based on the results of these tests, appropriate statistics to measure central tendency and variance can then be applied. At this point in the program, statistical analysis of trace constituent results is not warranted. Detected results will continue to be compared to water quality standards.

CONCLUSIONS

• A well-designed database information system can be an integral part of a dynamic groundwater-quality monitoring program. Monitoring data can be efficiently condensed, summarized and analyzed to assist in determining the effects of effluent recharge on ground-water quality and planning future monitoring strategy.

• General mineral analysis suggests that monitoring wells along the Santa Cruz are generally sampling recharged effluent. Monitoring efforts on background wells will be increased, along with analysis and interpretation of chloride/bromide ratios to help substantiate this conclusion. This data will also provide a more thorough characterization of groundwater along the Santa Cruz River.

• A complex pattern of nitrate concentrations among the 12 monitor wells was detected. Possible seasonal differ-

ences were also noted. Quarterly sampling will continue for nitrate and other general minerals, to allow statistical analysis of data. Nitrogen isotope analysis will be initiated at high nitrate wells to help identify the source of nitrate in the groundwater.

• Trace-constituent analyses indicated that recharged secondary treated effluent is not causing trace-contaminant pollution of groundwater along the Santa Cruz. If the trend continues, annual monitoring for trace organics can save money or provide funds for other aspects of the groundwater monitoring program.

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A SOFTWARE PACKAGE FOR ANALYZING WATER QUALITY DATA ON MICROCOMPUTERS

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INTRODUCTION

Statistical analysis of water quality data is becoming a routine part of many water quality regulation, management and remediation programs. Microcomputers and commercially available software packages are widely used for such purposes. However, many organizations are finding it difficult to effectively extract and utilize statistical information from monitoring data. Particularly troublesome is the fact that most available statistics software is fairly expensive, cumbersome to use for routine data analysis, and assumes a rather high degree of statistical expertise on the part of the user.

In an effort to overcome these difficulties, Colorado State University has developed a microcomputer statistics package specifically tailored to water quality data analysis. The package, called WQStat II, requires an IMB-PC compatible computer with hard disk and 640K RAM. Hercules, CGA, EGA, and VGA graphics are supported for screen displays. Hard copy graphics may be obtained via "Print Screen," provided that the printer in use supports graphics "screen dumps."

CAPABILITIES OF WQStat II

WQStat II is a self-contained data management and data analysis system designed for water quality management professionals with a moderate level of statistical training. The program is menu-driven, requiring no commands. WQStat is not an expert system per se. However, the software does incorporate a high level of statistical expertise by including only those data analysis tech-

niques which are most appropriate for water quality management and organizing them according to the most common information objectives of water quality monitoring programs. Those objectives are the following:

(1) Describing the distribution of water quality variables of interest

(2) Testing for significance of gradual trends in water quality over time

(3) Comparing the central tendency (mean or median) of two or more groups of data over time or space

(4) Evaluating the significance of extreme values or excursions

The program additionally provides information to the user who may be unfamiliar with some of the statistical procedures via "Consult the Expert" options in many of the menus. In some cases the "Expert" uses simple rules to guide the user in choosing and interpreting results from available statistical routines.

WQStat relies heavily upon graphical and nonparametric (not assuming a normal distribution) procedures in order to obtain the greatest possible applicability to water quality data. No details of these methods are presented in this brief discussion. Users will generally wish to consult references cited in the users manual for statistical background material. Among the more useful are Conover (1980) and Gilbert (1987).

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Date Management

WQStat II uses a data management system in which water quality observations for a single variable and location are associated with a single user-defined file name. The program provides a template for manual data entry and editing. Data can also be imported from ASCII files or Lotus 1-2-3 spreadsheets.

Observations can be entered at any frequency from quarterly to daily and need not be evenly spaced in time. However, WQStat II will prepare data for analysis by creating either a monthly or quarterly record according to the user's specificiations. "Quarters" are user-defined to correspond to seasons and need not be three months long.

When preparing data for analysis, WQStat II presents the user with a time series plot of the monthly or quarterly series. The user can select any desired segment(s) of the series for analysis using arrow keys to move an indicator pointer on the screen.

Summary Statistics

WQStat II provides the following summary statistics options for investigating the general distribution of a water quality variable.

(1) Mean, standard deviation, skewness, and kurtosis with tests for normality

(2) Time series plot

(3) Seasonal box-and-whisker plot (as an indicator of seasonal variation)

(4) Annual box-and-whisker plot (as an indicator of time trend)

(5) Histogram

(6) Correlogram (as an indicator of serial correlation)

(7) Kruskal-Wallis test for seasonality.

Trend Analysis

WQStat II offers two options for trend analysis on a selected data segment:

(1) Kendall-tau and Seasonal Kendall tests

(2) Analysis of covariance on ranks of data.

Both tests are performed at the 95, 90 and 80 percent confidence levels.

Median Analysis

The following median analysis options provide a comparison of average conditions across two or more sets of data.

(1) Wilcoxon signed rank test for comparing two data segments which can be paired

(2) Mann-Whitney test for comparing two data sets which cannot be paired

(3) Kruskall-Wallis test for comparing three to twenty data segments simultaneously.

Excursion Analysis

WQStat II provides two options for evaluating the significance of extreme values. First the program can compute the fraction or proportion of observations in each season which exceed some specified action level. Confidence limits (99% and 95%) are then given for those proportions.

The second option computes tolerance intervals, by season, for a specified segment. A tolerance interval on the differences between two files (locations) may be used to check for impacts on one location (say a downgradient well) with respect to another

(say an upgradient well). The user may select either parametric (assuming a normal distribution) or nonparametric (distribution-free) tolerance intervals.

SUMMARY, AVAILABILITY AND TERMS OF USE

WQStat II provides a user-friendly environment for statistical analysis of water quality data on microcomputers. The statistical expertise required of users is minimized through incorporation of appropriate (nonparametric and graphical) data analysis procedures, organizing the procedures according to information objective, and "help" screens provided through "Consult the Expert" options.

The software and users manual may be obtained from the author. Send checks only payable to Colorado State University for $20 to cover the expenses associated with its dis-

tribution. WQStat II is copyrighted but not copy protected.

You are free to use, copy and distribute WQStat II if no fee is charged for use, copying or distributing and WQStat II is not modified in any way.

Colorado State University makes no warranties, expressed or implied, including, but not limited to, merchantability or fitness for any particular purpose. In no event shall Colorado State University or its employees be liable for indirect or consequential damages arising from the use of the software program.

REFERENCES

Conover, W. J. 1980. Practical Nonparametric Statistics. John Wiley and Sons, Inc., New York. 493 pp.

Gilbert, R. O. 1987. Statistical Methods for Environmental Pollution Monitoring. Van Nostrand Reinhold Co., New York. 320 pp.

Case Studies

THE DEVELOPMENT AND IMPLEMENTATION OF AN INVESTIGATION INTO THE SOURCE AND EXTENT OF SEDIMENT CONTAMINATION IN AN ISOLATED ARM OF LAKE TRUMAN, MISSOURI

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ABSTRACT

A Special PCBs Study, which provided for intensive water, sediment, and fish-tissue sampling, was conducted by the U.S. Environmental Protection Agency, Region VII at twenty-four sites on fifteen water bodies in the Kansas City, Missouri area. As a result of this survey, an isolated arm of Lake Truman near Clinton, Missouri, was identified as having atypical PCB sediment contamination. A follow-up survey was therefore proposed, designed, and implemented in order to determine the extent and source of the detected contamination.

This paper addresses the development of the follow-up survey, which incorporated the results of the first study, historical and geographical information on the site, point and non-point source contributions, and the availability of numerous sediment transport mechanisms. It also discusses the study design, the fish and sediment-sampling methodology employed, and the results of data review and analyses. The tools used to develop and implement this study are reviewed for their potential application in general water quality network design.

INTRODUCTION

In November 1987, U.S. Environmental Protection Agency (EPA) Region VII personnel designed and implemented a sampling survey to evaluate polychlorinated-biphenyl (PCB) levels at twenty-four sites on fifteen water-bodies in the Kansas City, Missouri, area. The survey, which included physical detection methods and the collection and analysis of water, sediment, and fish tissue samples, was conducted in response to the public concern raised over allegations that PCB-contaminated materials had been dumped into several area lakes and streams. None of the evidence gathered during the survey supported those allegations. However, the fish tissue and sediment samples from a Lake Truman, Missouri, survey site were found to have atypical PCB concentrations. In order to determine the extent and source of the detected contamination, an additional sampling survey was proposed, designed, and implemented.

BACKGROUND

Beginning in December 1984, Mr. John Moran, Jr., a former employee of C.B. Oil Company of Kansas City, Missouri, made a series of allegations that he and other employees of the company had dumped PCB-contaminated capacitors and PCB-contaminated oils into a number of water-bodies in the Kansas City, Missouri, area. In response to those allegations, investigations were launched by EPA Region VII, the EPA Office of Criminal Investigations of the National Enforcement Investigations Center, the Federal Bureau of Investigation (FBI), and a subcommittee of the U.S. House of Representatives. At each stage in the investigations, Mr. Moran named additional alleged dump sites and changed various aspects of his account. During an interview

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conducted by the FBI on April 16, 1987, Mr. Moran stated that his account of the alleged PCB-dumping incidents had been a fabrication. He was subsequently indicted on federal charges of making false oral and written statements to federal investigators.

Although Mr. Moran's statements were not corroborated at the trial, he was acquitted of those charges in Federal District Court on October 22, 1987, thereby raising questions about the safety of the waters in the Kansas City area. Consequently, in November 1987, a study plan was designed and implemented by EPA Region VII to assess PCB levels in area waters. The plan incorporated information taken from court testimony and site reconnaissances to provide for an intensive sampling and physical detection survey for PCBs and capacitor materials in twelve waters that Mr. Moran identified as alleged dump sites, at two background sites, and at several additional locations of public interest. These locations are depicted on the Map of Figure 1.

None of the evidence collected during the study supported Mr. Moran's dumping allegations. No PCBs were detected in any of the water samples, and no capacitor materials were found in the intensive diving and metal detection studies. With only one exception, the PCB levels detected in sediment and fish tissue analyses were consistent with those typically found in area waters. The only study site at which atypical PCB levels were detected in fish tissue and sediment is on Lake Truman at the terminus of an old county road south of Clinton, Missouri and east of Missouri Highway 13 (Figure 2). The results of the sediment survey at this site are provided in Figure 3. Analyses of whole carp samples collected at this location showed PCB contamination of 1.1 ppm.

The degree and pattern of contamination found at this Lake Truman sampling site (hereafter referred to as the "Site") made it clear that the source of contamination was not the dumping of PCB materials as described by Mr. Moran. The data did not, however, provide sufficient information to determine the source and extent of the detected contamination. Consequently, an additional sampling

survey was proposed, designed, and implemented to address those issues.

DEVELOPMENT OF STUDY PLAN

Establishing study goals was the first step in developing the Lake Truman study plan. Based on the results of the first study, a problem had already been identified, namely PCB contamination in the sediment and fish of an isolated arm of Lake Truman. The questions that needed to be addressed by the follow-up study were:

1. What caused the contamination, and is it an active source?

2. What is the extent of the PCB contamination?

The second step was the identification and use of available resources to answer those questions. In order to identify possible sources of the contamination, information on present and past Site use was required.

Lake Truman is a man-made lake, owned by the federal government and operated by the U.S. Army Corps of Engineers (COE). Therefore, records on the development of the lake were available and were reviewed. County and state maps, aerial photographs, and industrial directories were also reviewed, and representatives of the Corps of Engineers and the City of Clinton were interviewed to acquire Site information that had not been committed to record. The following information was collected from these sources.

General History of Lake Truman

Construction of Lake Truman began in the 1960s. The lake is used for flood control and recreational purposes and as a drinking water supply for two communities in Henry County, Missouri.
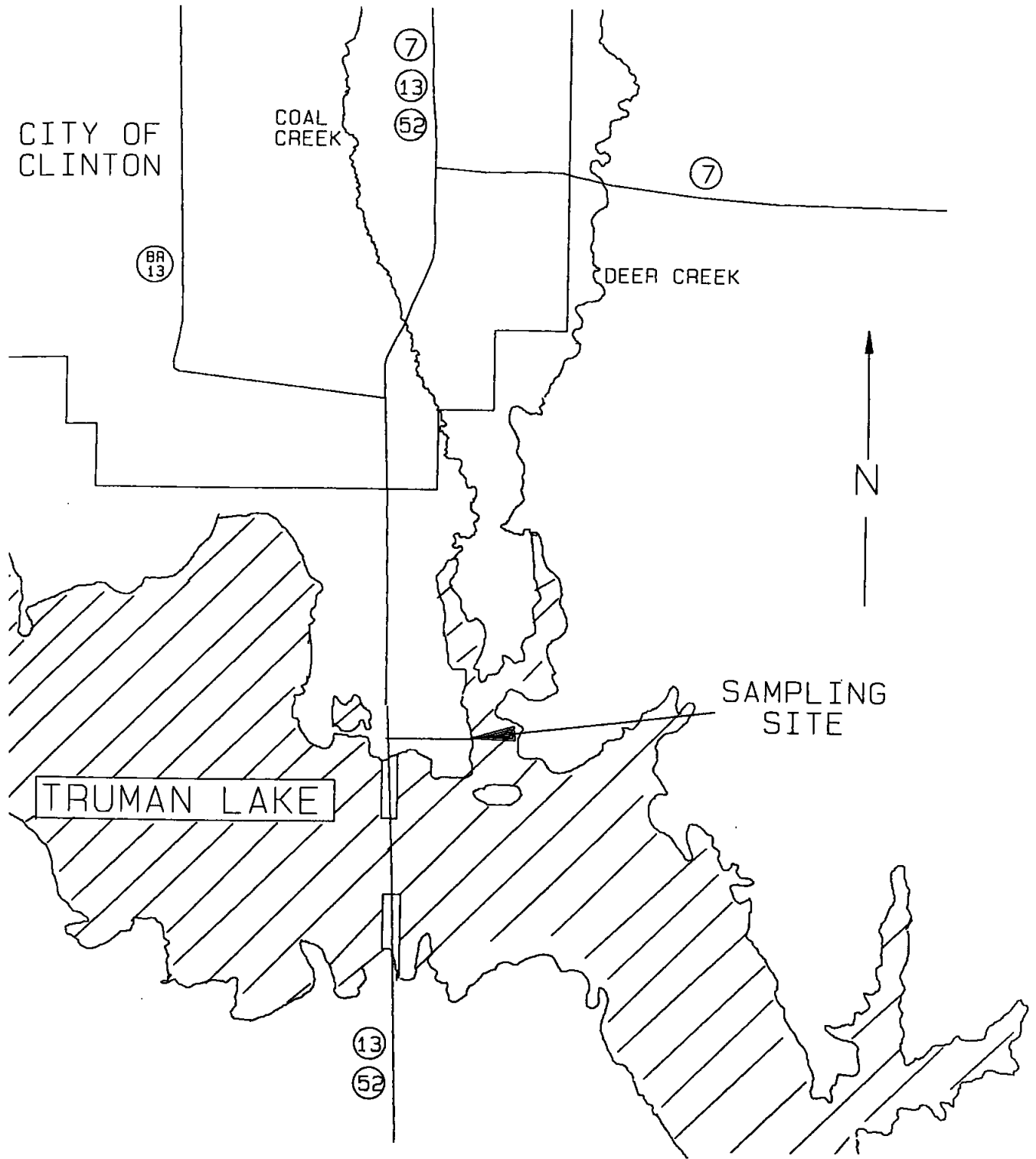
Site Description

The Site is located on Tracts 12720 and 12715 in Township 41, Range 26, Section 24 of Henry County, which are owned by the U.S. Government as a flood relief area within the design flood pool of Lake Truman. The Site

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FIGURE 1
SAMPLING LOCATIONS
FOR THE
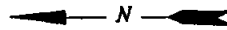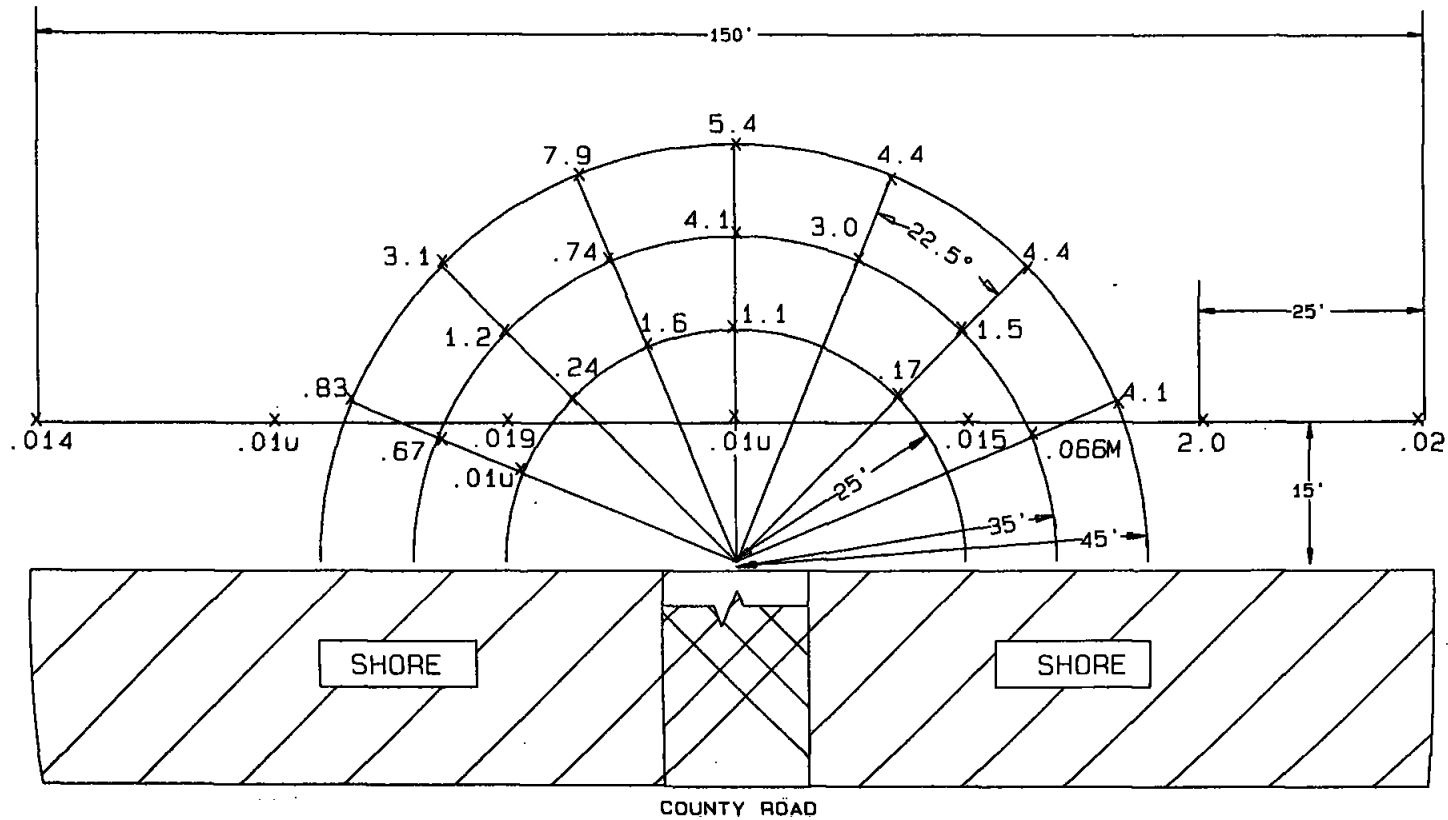SPECIAL PCBS STUDY
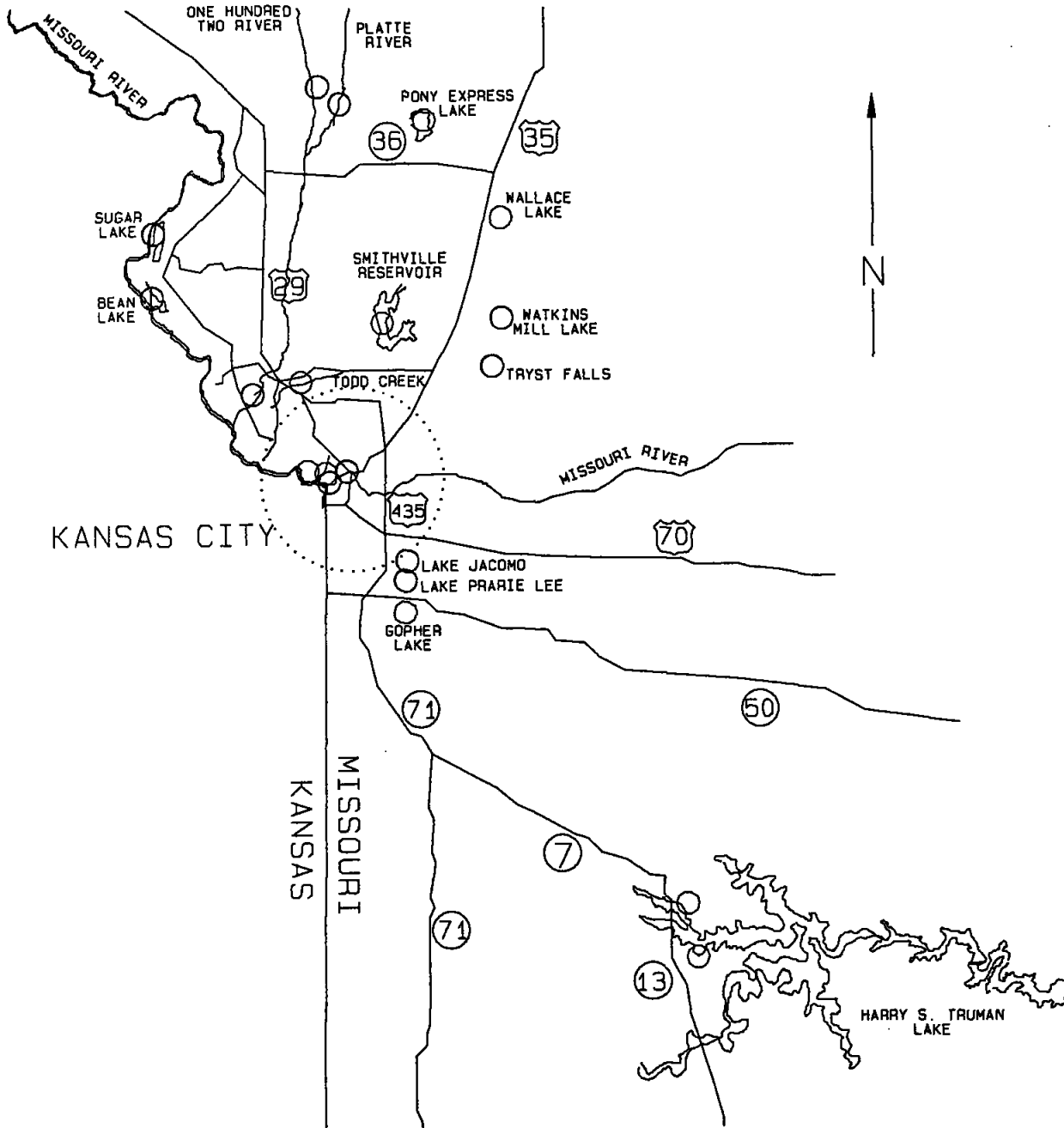
TRUMAN LAKE
SAMPLING SITE
FIGURE 2

PCB LEVELS IN LAKE TRUMAN SEDIMENT (ppm)
FIGURE 3

KEY

SAMPLING POINT	x
UNDETECTED	u
COMPOUND WAS QUALITATIVELY INDENTIFIED: HOWEVER, CONCENTRATION WAS TOO LOW TO ESTABLISH THE QUANTITATIVE CONCENTRATION	M

is defined by the terminus of an old county road (hereafter referred to as the "Site county road") that extends east of Missouri Highway 13 at a point approximately 2.6 miles south of the intersection of Highways 13 and 7.

Site Land-Use History

The Site county road was inundated by Lake Truman in 1979 and is now partly submerged. Prior to 1971, the land on which the site is located was owned by two private parties and was apparently used for agricultural production. In 1971, the land was purchased by the U.S. Government and incorporated into the design flood pool of the lake. Inundation of the lake at this location resulted in the development of a lake arm that extends from the main body of Lake Truman north toward Clinton, Missouri. This lake arm receives the discharges of two streams: Coal Creek and Deer Creek.

Site Activity History and Possible Contamination Source Hypotheses

The information acquired on historic Site activity indicated that there were a number of possible sources of the detected PCB contamination. The background information collected on each of these possible sources is provided below.

a. Transformer Spill or Explosion

U.S. Army Corps of Engineers (COE) aerial photographs taken of the Site and surrounding area showed that three rural residences were located on the Site county road. Each of the residences that had electric service would most likely have had a transformer posted on its service line. COE photographs indicated that utility poles were posted along the northern edge of the county road. Although the resolution of the photographs impeded the confirmation of all utility pole locations, several poles were easily identified. Their spacing indicated that a utility pole may have been posted about 45 feet east of the county road where it ends at the shoreline. It was noted that this location approximately corresponds to the location of the sample that contained the highest PCB

concentration detected in the original sampling survey.

COE records show that the Site area fell under the jurisdiction of the Osage Valley Electric Co-op (OVEC). Information in the COE - OVEC Utility Relocation Contract confirms that OVEC-owned utility lines were posted along the Site county road prior to the lake's inundation. Those lines were removed at a date not specified in the 1976 contract. However, due to the construction of the lake, it appears that they would have been removed prior to the lake's inundation and after the establishment of the contract (i.e. between 1976 and 1980). If a transformer was posted on a pole in the Site area, and it leaked or exploded before or during removal, it may have been the source of the detected contamination.

b. Road Oiling

Road oiling for dust suppression is a common practice in rural areas. Because the Site county road is a dirt and gravel road, it is possible that the road was, in the past, sprayed with oil. Waste oils have often been used for that application, and there are a number of documented cases in which environmental contamination has occurred from the road application of contaminated waste oils.

Review of the COE aerial photographs revealed the presence of discolored soils along the length of a farm residence access road near the Site. This road appeared to be darker in color than other area roads, suggesting the possibility of road oiling. If any area road were sprayed with PCB-contaminated oil, the spraying could account for the detected contamination.

c. Missouri Highway 13 Construction

Missouri Highway 13 was built in the mid-1960s. A COE aerial photograph taken in 1966 shows that land on both sides of the Site county road was used as a borrow pit during the construction of the highway. Aerial photographs taken after 1966 also show uneven vegetation at the borrow pit locations. Although PCB contamination from

construction activities appeared to be improbable, spills of PCB contaminated hydraulic fluids used in construction equipment, and/or the use of PCB-contaminated oils for borrow pit or road dust suppression, could have resulted in the detected contamination.

d. Capacitor Spill or Explosion

PCBs were at one time used in very high concentrations in the dielectric fluids of capacitors, which are typically found posted along utility lines and are used to maintain steady currents along the line. Although the PCB Aroclor (PCB-1260) detected at the Site was not typically used in capacitors, the weathering and degradation of capacitor oils over an extremely long period of time could potentially result in the type and level of contamination found. As discussed earlier, COE contracts and aerial photographs indicate that utility poles were posted along the Site county road and would have been removed from service at some time after 1976 and before 1980. If a capacitor had been posted on a utility pole near the Site, and it leaked or exploded, it could have resulted in the detected contamination.

e. Clinton Wastewater Treatment Plant

Coal Creek flows into the Lake Truman arm in which the sampling Site is located. This creek receives discharges from the Clinton Wastewater Treatment Plant (WWTP), an activated sludge treatment plant that went on line in 1981. , Prior to the plant's construction, the Clinton treatment facility was a two-stage settling pond at a location 1/4-mile northwest of the present plant. It served the eastern half of Clinton and also discharged into Coal Creek. If PCBs had been present in the discharge of either of these facilities, they could have contributed to the contamination detected at the Site.

f. Junkyard Operations

Interviews with representatives of the City of Clinton resulted in the identification of two abandoned junkyards within the vicinity of the Site. The first of those junkyards was reportedly located in the southeastern corner

of the northern Highway 13 borrow pit. The second was reportedly located near the intersection of the abandoned Missouri-Kansas-Texas railroad tracks and the first county road north of the Site county road. If PCB-contaminated materials were handled at either of these locations, they could have contributed to the contamination detected at the Site.

In addressing the issue of contamination distribution and extent, field limitations needed to be recognized in terms of the practical scope of the sampling survey. By reviewing the geographical information on potential sources and the data collected in the original study, the possible extent of PCB contamination was evaluated. That information was applied in the selection of proposed sample collection locations. Table 1 lists these locations and the rationale used in their selection.

In addition to the sediment collection efforts, fish tissue sampling was proposed to assess the level of PCB contamination in the edible portions of game and bottom-feeding fish near the Site.

Figure 4 illustrates the general sampling locations proposed for the immediate Site area. Block numbers for eleven of the locations were assigned for reference. In addition to the sampling locations depicted on Figure 4, samples were proposed for the Coal Creek Bed at points immediately downstream and upstream of the former wastewater treatment lagoons and at the creek's point of intersect with Lake Truman. Samples were also proposed for the two Henry County drinking water supplies, the Clinton WWTP, the Deer Creek bed, and from the two locations that Clinton officials identified as abandoned junkyards.

Because the area over which samples were to be collected was extensive, a large number of sampling locations were required to define it. Therefore, composite sampling methods were proposed in order to conserve laboratory resources. For each of the blocks defined in Figure 4 (with the exception of Block 9 and a portion of block 10), it was proposed that a number of sub-samples be collected and that

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TABLE 1. RATIONALE FOR SAMPLE LOCATIONS

LOCATION	RATIONALE
The Coal Creek Bed	To evaluate the current and former Clinton Wastewater Treatment Facilities as possible sources
Clinton WWTP Sludge	To evaluate the current Clinton WWTP as a possible source
Borrow pit (low point)	To evaluate possible contribution from Hwy 13 construction
Submerged length of the Site county road	To evaluate possible contribution from road oiling / capacitor or transformer explosion
West end of Site county road at the next lake arm to the east	To evaluate possible road oiling contamination
Abandoned farmhouse road	To evaluate possible road oiling contamination
Samples in identified area of contamination	To characterize contaminated area more fully
Split-core samples in identified area of contamination	To determine the sediment depth at which maximum PCB contamination occurs
Site lake arm inlet	To determine the extent of the contamination
South, north, and east of the original grid	To determine the extent of the contamination
Henry Co. and Clinton Drinking Water Treatment Plants	To determine if PCBs are present in the Lake Truman drinking water supplies
The Deer Creek Bed	To collect background information on the Site
Suspected abandoned junkyards near Site	To determine if either contributed to the contamination

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SAMPLING BLOCKS AT TRUMAN LAKE
FIGURE 4
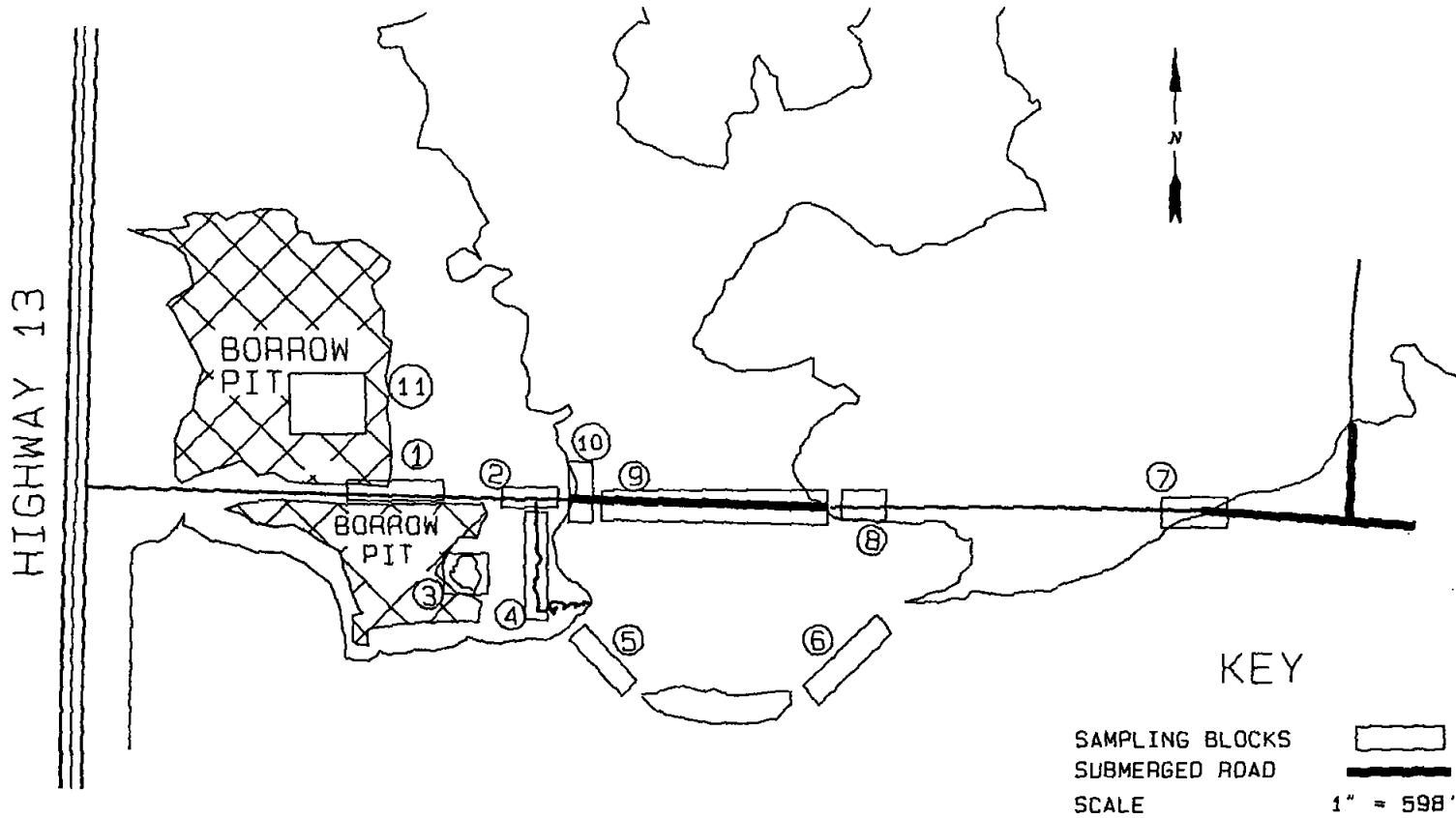
a portion of each sub-sample be composited into a single sample for that block. An analytical strategy was developed that called for PCB analyses of these composite samples first and the retention of the sub-samples for re-evaluation upon receipt of composite sample data. If the level of PCB contamination in a given composite sample multiplied by the number of its sub-sample aliquots exceeded 2.0 ppm, that composite's sub-samples were to be submitted for analyses. The selection of the 2.0 ppm criteria was based on the action level established for PCBs in contact with drinking water. The sampling plan also established that this criteria be used in evaluating all data collected during the survey.

In all, the collection of 40 discrete samples, 84 sub-samples, 15 composite samples, and 9 split-core samples was proposed. Duplicate samples, field blanks, and equipment rinsates were also included for quality-control purposes.

IMPLEMENTATION OF STUDY PLAN

Samples from the Clinton Wastewater Treatment Plant and the Henry County Drinking Water Plants were collected in January 1988. Due to lake-level fluctuations and the desirability of sampling at the same lake stage as the original survey, the remainder of the follow-up survey was put on hold until the lake level was suitable. The week of May 31, 1988, the lake elevation was comparable to that of the original study and the sampling survey was initiated. From May 31, 1988, to June 2, 1988, Region VII personnel collected the samples as outlined in the study plan and illustrated in Figure 4. The reference shoreline for the study was defined as a line 7 feet west of and parallel to the true shoreline so that it approximated the shoreline used during the original study.

The sample location designated as Junkyard #2 in the sampling plan was not sampled at the time of the survey. That location was investigated and was found to be dedicated to agricultural production. Due to the soil disturbance and displacement associated with tilling, any soil samples taken from this location would have been unrepresentative and therefore were not collected.

DATA SUMMARY AND ANALYSES

WATER

Analyses of the samples collected from the two Henry County Drinking Water Plants and the Clinton Wastewater Treatment Plant found no PCBs in the raw or treated water at the plant.

FISH

Samples of white crappie, largemouth bass, and carp were collected from the area immediately surrounding the Truman Lake Site. Fillets of each species were prepared and analyzed. The PCB concentrations detected in the samples were 0.17, 0.23, and 1.2 ppm respectively. In addition to the fillets, a whole carp sample was collected and analyzed. PCBs were detected in that sample at a level of 1.8 ppm.

The primary interest in sediment contamination stems from its effect on the food chain. That effect is best assessed by the sampling and analyses of fish. The U.S. Food and Drug Administration has established an action level of 2.0 ppm for PCBs detected in the edible portion of fish (e.g., if the PCB concentration in fish fillet exceeds 2.0 ppm, advisories may be issued which limit or ban consumption). The concentrations in the fillet samples were elevated but below the FDA action level. The PCB concentrations in the whole carp samples collected during this study and the November 1987 study (1.8 and 1.1 ppm, respectively) were also below the action level. Whole carp samples taken in November 1987 at a location approximately 2 miles south of the subject arm (nearer to the lake's main basin) had PCB concentrations approximately one one-hundredth of the FDA action level. A comparison between the results at the two sites, however, indicates that the elevated PCB levels in the fish collected from the study site are due to the contamination found on the Site county road. Furthermore, the difference between the PCB concentrations in the fish collected in November 1987 and May 1988

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suggests that PCB levels may be increasing in the subject-arm fish. This disparity may also be due to the analytical variation inherent in fish tissue analyses. To ensure that future PCB concentrations would not exceed the action level and go undetected, annual or biannual collection of fish in the subject arm was recommended. During the first quarter of FY89, the Water Monitoring Section of the EPA Region VII Environmental Services Division performed a fish sampling survey on three areas of Lake Truman, including the subject arm. The results of that are expected to be finalized by July 1989.

SEDIMENT

The results of the sediment sample analyses are provided in Figures 5, 6, 7, and 8. No PCBs were detected at the mouth of the lake arm, indicating that the contamination is localized and that the main body of Lake Truman is not affected. In addition, the absence of PCB contamination in the samples collected from Site tributaries, Coal and Deer Creeks, eliminates the Clinton WWTP and other upstream discharges from the list of possible contamination sources. The highest PCB concentrations detected during the survey were found in the samples taken directly from and in the near vicinity of the Site county road. PCB levels ranged from 10 ppm to 0.023 ppm in the composite samples taken from the dry portion of the county road and from 7.5 ppm to non-detected in the samples taken from the submerged portion of the road. The pattern of PCB concentrations in the road samples indicates that the contamination is highest at the western end of the road and decreases eastward as the road passes through the lake. Furthermore, PCB concentrations in the terrestrial and aquatic samples taken from areas on either side of the county road show that the level of contamination generally decreases as the distance from the road increases.

The pattern and degree of the PCB contamination detected at the Site indicate that the source is either historic road oiling or a spill of utility dielectric fluid. The dispersal patt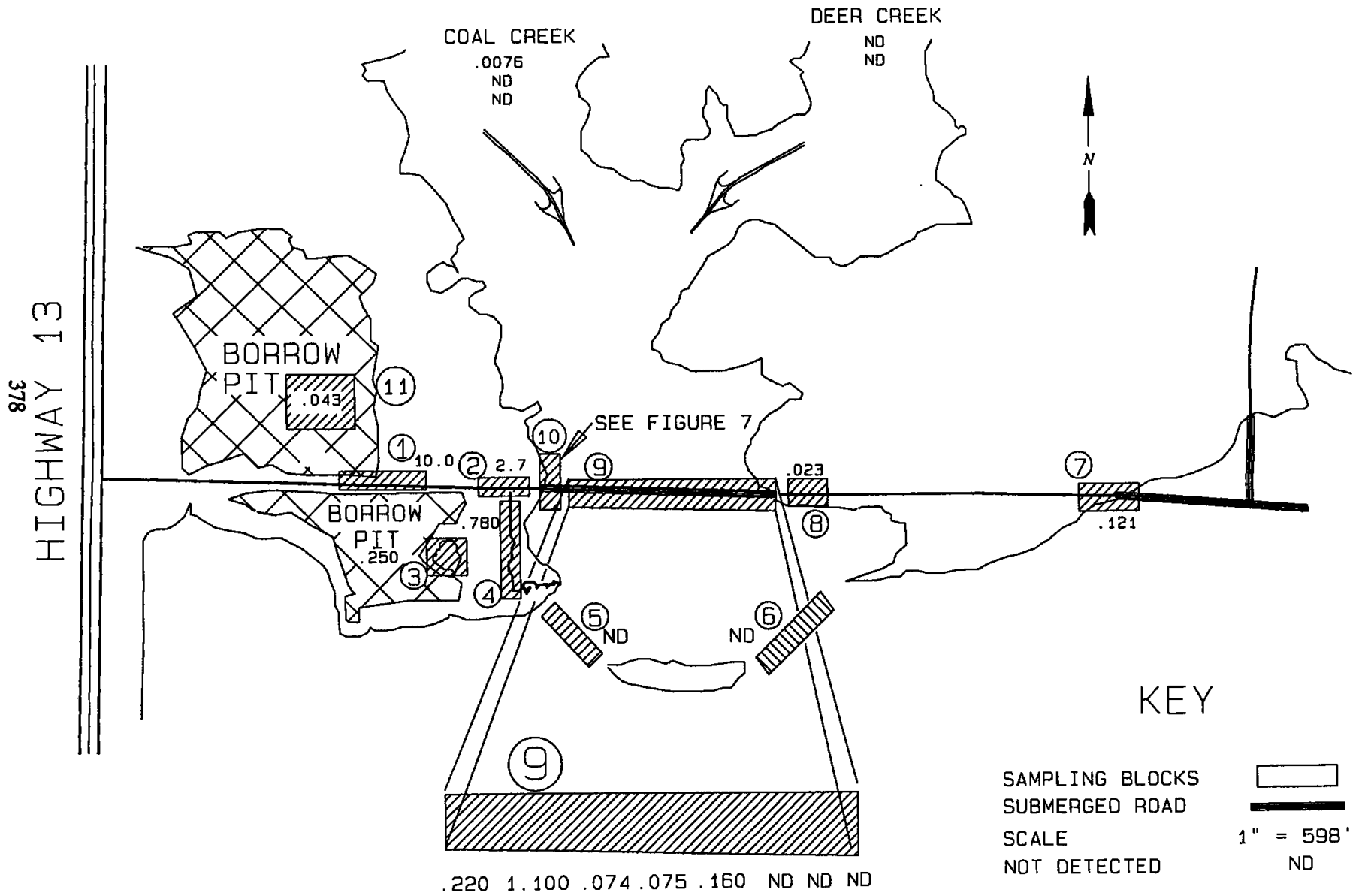erns and the depth at which PCBs were detected in the lake sediment (4 to 6 inches), suggest that the contamination has been present for a number of years. The composite sample that showed highest contamination was taken from an area approximately one-thousand feet inland from the lake's recreational or normal elevation shoreline. PCB-contaminated sediments have traveled in a down-gradient eastward direction via the transport mechanisms of vehicle traffic, stormwater runoff, and lake-level fluctuations. In addition, water currents in the lake have provided another transport mechanism, which has resulted in the mixing of contaminated surface sediment with deeper lake sediment and has caused the relatively widespread but low-level PCB contamination detected north, south, and east of the county road and the original sampling area.

Because the highest PCB concentration (10 ppm) was detected at the western-most point on the sampled county road, it is possible that similar or higher levels exist west of this location. Further sampling would be required to determine whether this is the case. Because the lake is under the jurisdiction of the U.S. Army Corps of Engineers, the information collected during this survey was forwarded to the COE Kansas City, Missouri, office for additional evaluation.

CONCLUSIONS

The information collected during this survey enabled the investigators to answer the questions posed on the source and extent of PCB contamination detected in Lake Truman sediment. The distribution and level of contamination shows that PCBs were introduced at the site prior to the development of the lake at that location. In addition, the data indicated that the contamination was due to either road oiling with PCB- contaminated oils or a spill of utility dielectric fluid. Information on the extent of the contamination enabled the investigators to identify its northern, eastern, and southern boundaries and shows that the contamination is localized and does not affect the main body of Lake Truman.

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FIGURE 5

COAL CREEK
.0076
ND
ND

DEER CREEK
ND
ND

N

HIGHWAY 13

378

BORROW PIT
.043 ⑪

① 10.0 ② 2.7 ⑩ SEE FIGURE 7 ⑨ .023 ⑦

BORROW PIT
.250 .780

⑧

③ ④ .121

⑤ ND ⑥ ND

⑨

.220 1.100 .074 .075 .160 ND ND ND

KEY

SAMPLING BLOCKS
SUBMERGED ROAD
SCALE   1" = 598'
NOT DETECTED   ND

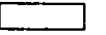# BLOCKS 1, 2, AND 4 SUB-SAMPLE CONCENTRATIONS (ppm)

FIGURE 6
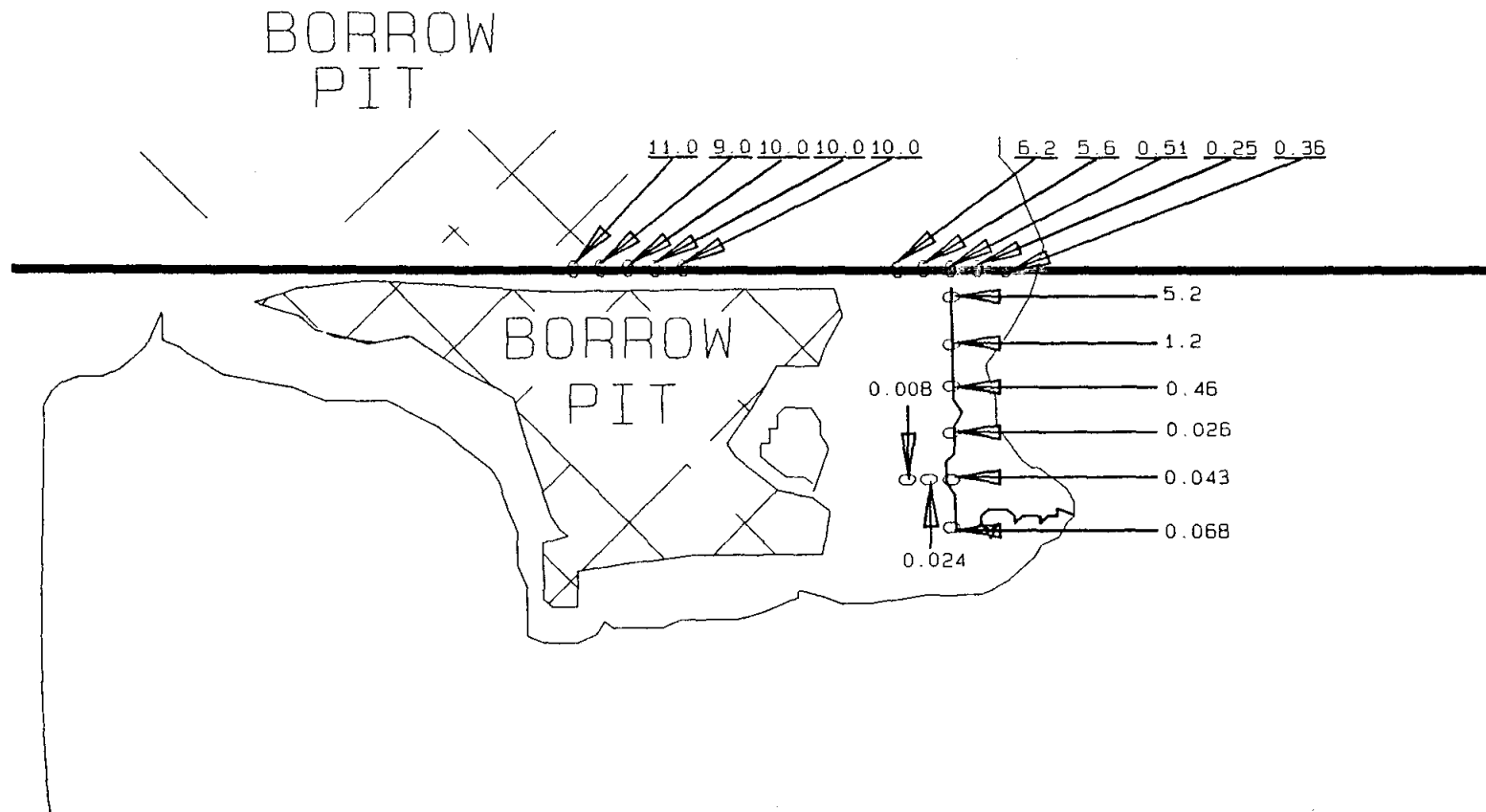
FIGURE 7

KEY
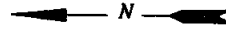
SUB - SAMPLE ○
DISCRETE SAMPLE ▱
SPLIT - CORE SAMPLE △
COMPOSITE SAMPLE ▭

380
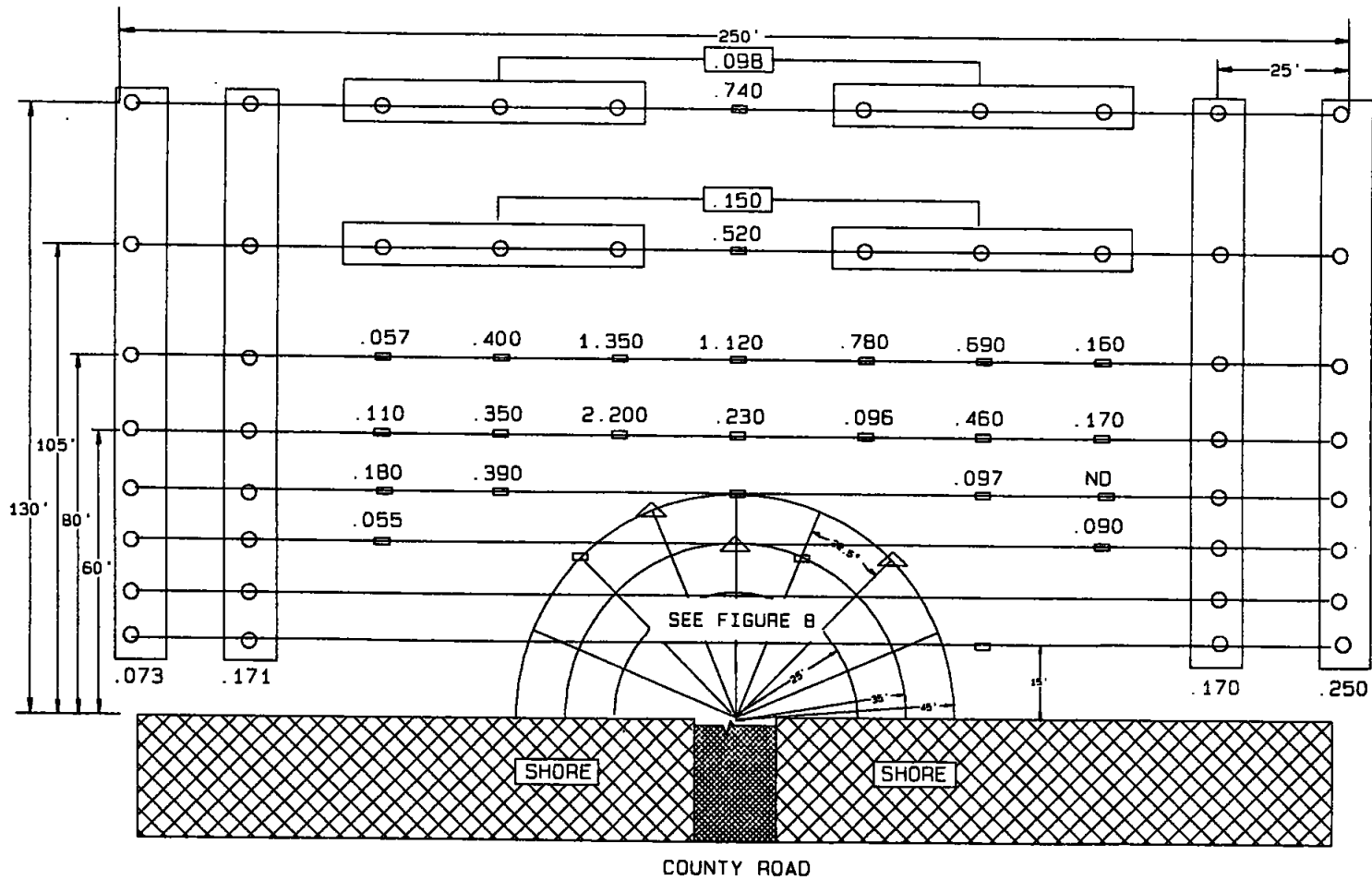
BLOCK #10 SUB-SITE PCB LEVELS (ppm)
FIGURE 8
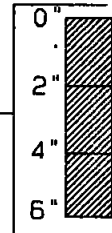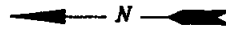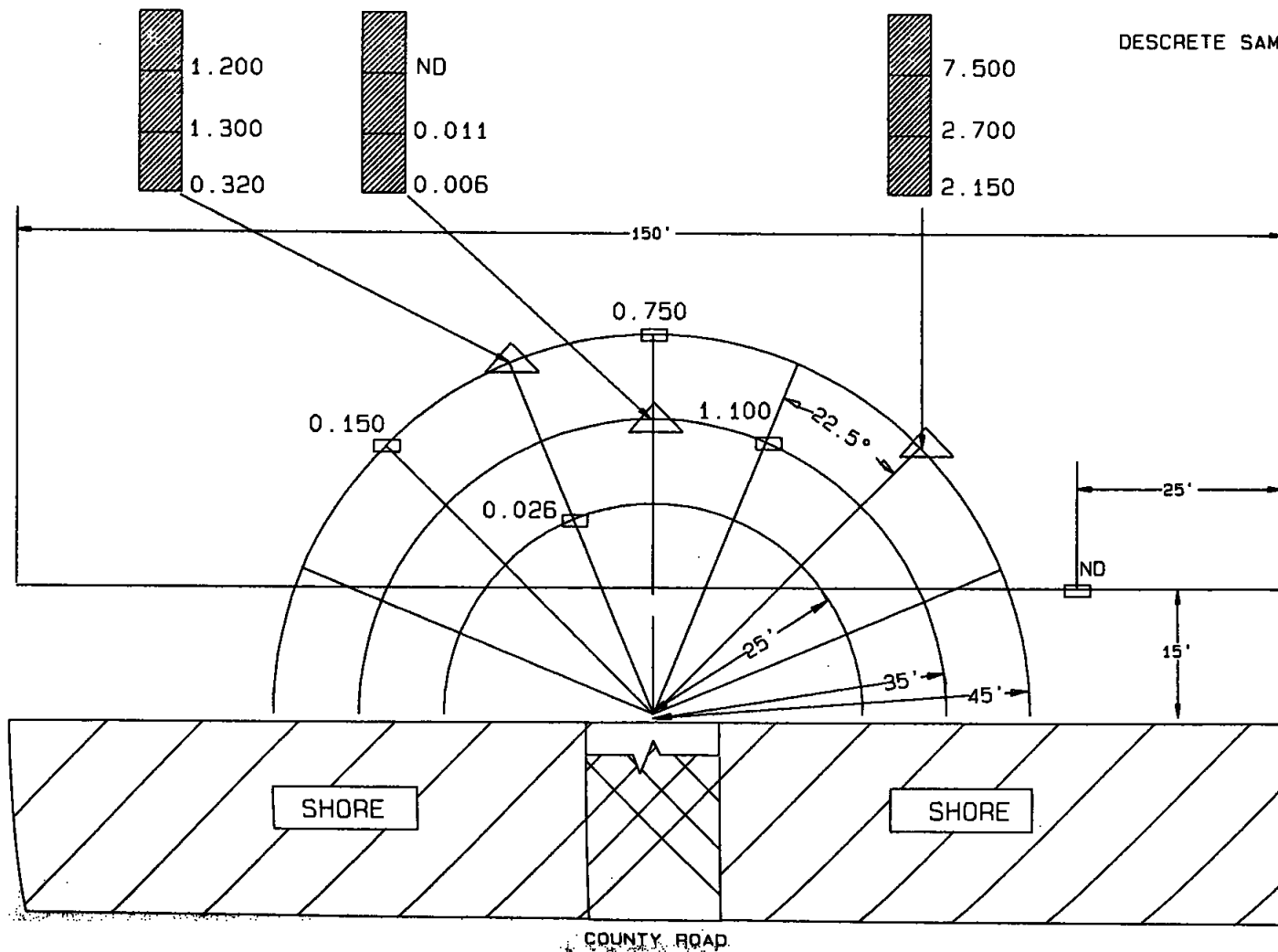
GIS APPLICATIONS IN MANAGEMENT OF NONPOINT SOURCE CONTROL PROGRAMS

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Phoenix, AZ 86384

BACKGROUND

The world is a glorious bounty. There is more food than can be eaten, more children than we can love, more laughter than can be endured, more wisdom than can be absorbed. Canvas and pigments lie in wait, stone, wood, and metal are ready for sculpture, random noise is latent for symphonies, and yet, the world is finally unknowable.

(McHarg, 1971)

Like McHarg in his book Design with Nature we are confronted with an abundance of information; our task is how to make sense of it.

In my position as manager of the Nonpoint Source Program in the Arizona Department of Environmental Quality, I have encountered the same problem (too much information in some areas causing problems with interpretation and too little information in other areas necessitating best judgement calls by experts in the field). Our short-term goal in the Office of Water Quality is to develop a computer system to locate, analyze and predict the effects of man's activities on the water quality of the State. Hopefully this short-term goal will serve to achieve the ultimate mission of the Department to develop programs to protect, preserve and enhance environmental and public health of Arizona. My purpose in this presentation is to: 1) Describe the logic for the Department's choice of a Geographic Information System (GIS) as a tool for managing Nonpoint Source Pollution; 2) Convey the basics of how a GIS system works; 3) Provide information on the problems we encountered in the system development; and 4) Propose options for the system use in the future.

Managing nonpoint sources of pollution in order to minimize impacts to water quality is complex technically, politically, socially and economically. Basically a nonpoint source management program must prioritize various environments (watersheds) by how tolerant or intolerant they are to human use; and then develop methods and mechanisms to modify the use of the land to minimize impacts to the environment and water quality.

A computerized system was determined as the only efficient way to compile the data necessary to manage nonpoint sources of pollution. Water quality and quantity have been impacted as natural and man-made forces have altered vast arid and semi-arid watersheds. Cultural and environmental forces have combined to cause alterations in the hydrologic system. The physical components and human cultural practices are inherently spatial and variable throughout the watersheds. Variations in precipitation, vegetative cover and soil type are distributed across the landscape as well as the differential landuse practices which operate on them. In response to the needs of land planning and resource assessment, Geographic Information Systems have been developed over the past two decades with which to evaluate and analyze the spatial aspects of resources and processes. These GISs allow for the discrete assessment of geographic attributes for investigation of their spatial interaction and distribution.

Geographic Information Systems also provide for data transformations in terms of integration of both spatial and nonspatial attributes in modelling natural systems.

METHODOLOGY

The definition of a Geographic Information System is 'a system for the efficient input, storage, representation and retrieval of spatially indexed data'. This emerging technology of GIS is to map drafting and data interpretation as word processing is to the hand-written word. The idea of recording different layers of data on a single map dates back at least to the Revolutionary War, when a French cartographer prepared hinged overlays for troop movements at the battle of Yorktown. In 1855 a map of a cholera epidemic in London helped solve a public health crisis by pinpointing a contaminated well as the cause of the outbreak (Bylinsky, 1989).

Geographic Information Systems combine the functionality of computerized mapping applications and the power of data base management programs into a single integrated package. This allows users to retrieve data in any combination, produce maps at any scale or level of detail, and most important, query the data base by posing "what if..." questions. Scenarios can be created, situations modeled, and consequences of actions explored without actually implementing proposed actions.

Basically, map data is presented as either point, line or area (polygonal) information. The program we use, developed by Environmental Systems Research Institute, is called Arc/Info (Arc from the mathematical term and "information"). Arc/Info is viewed as a very complex package that takes a year to become proficient in its use. The software makes it possible to combine and manipulate geographical data from maps and numerical information about water quality analytical results or almost anything else that is pertinent to the problem. Satellite images are raster data, the same as the points displayed on a television screen. Data can be transferred from line to raster and back again or combined on one scene. An Erdas system

used in conjunction with Arc/Info allows a user to superimpose on a satellite image on a digitized map of the same area; thus making it easy to update line maps based on recent remotely sensed data.

In the near future, GIS will be an even more powerful tool in assessing the water quality of Arizona. Currently, the Arizona Department of Environmental Quality, the Arizona State Land Deparment, the U.S. Geological Survey (USGS), and others are creating the Arizona Hydrographic Information System. Hydrography for most of the State has been digitized by the USGS at a scale of 1:100,000. This data is now being processed to become a base used by multiple State and Federal agencies interested in water.

Since each stream reach or waterbody will have a STORET code and other attribute information tied to it, water quality for the entire state can be evaluated. In the relational data base files can be created that have water quality standards for streams and water bodies. Data files will have to be created containing all of the ADEQ's water quality data. Data from other agencies can also be accessed for the assessment of water quality and standards violations.

A computer program can be written that will automatically compare data files with the water quality standards files for each segment. The segments that have violations can be listed in the form of a tabular report and shown graphically on a plot that has the actual sampling sites and the reach that is in violation of some specific water quality parameter. The stream reaches that are in violation can be plotted in red to show that these reaches are not supporting the protected uses.

After identifying the streams and waterbodies with water quality problems, the GIS can be used to located any suspect sources that may be causing the problems. For example, if one wants to know what could be causing a problem in a certain area the GIS can bring back any source that is upgradient or slope within a zone of x miles on either side of the stream within a certain basin. A program can go into all existing

maps (landfills, wastewater treatment, mines, urban areas, vegetative communities, soil type, geology, etc.) and bring back in graphical or tabular form those possible sources (point and/or nonpoint) that fall within that range. The tabular data will contain any pertinent information about the source. Information could be the name of the mine, its location, the owner, etc. Any type and amount of information can be coded behind that geographic point or area.

APPLICATIONS

In theory, a Geographic Information System is very useful. Following are three case histories of how the GIS worked for the Department but also the problems that were encountered.

Nonpoint Source Pollution

The GIS system was used in the generation of Arizona's Nonpoint Source Assessment report. One of the elements of the report required by EPA was to identify those waterbodies that were not attaining water quality standards as a result of nonpoint source pollution. First the point sources had to be located to determine if they were causing the problems. Then the nonpoint sources were delineated by identifying the landuses across the State. Unfortunately information on landuse within our State is limited at best. Layers were generated at a scale of 1: 1,000,000 for the following landuse activities: irrigated agriculture, urban lands, grazing, silviculture, mineral districts, landfills and superfund sites. Upon determination of a water quality problem, the GIS system was utilized to identify the possible causes of the problem, be it either point source or nonpoint source. Although we were unable to use the detailed hydrography at the assessment stage, the system was used in our interpretation of the available data.

Hydrography

Development of the hydrography was another problem. As was previously described, hydrography in the State has been digitized by USGS at a scale of 1:100,000.

Problems have been encountered in utilizing the data because of line matching problems across map boundaries due to differing mapping criteria and digitizing methodology between mapping units. Each stream reach was to be labelled using EPA's Water Body System with associated files carrying the applicable water quality standards. The Reach File system was found to be over 50 miles off in some areas of our State and some stream segments identified were inaccurately listed in the stream hierarchy. Problems have also been encountered because of poor locational accuracy of EPA data. We still hope that monitoring data housed in the STORET system will be useful for identifying standards violations and to assess water quality in general.

Verde Basin

The GIS was used to evaluate management alternatives to protect water quality in the Verde Basin. The Verde Basin's waters are heavily used for recreation, have valuable riparian habitat, and are a major source of drinking water for the Phoenix metropolitan area. Various landuses contribute to nonpoint source pollution within the Basin. Sediments from sand and gravel operations have had a major impact on water quality and have threatened riparian habitat along the Verde River. The State Parks Department is actively acquiring land for a greenbelt along the river. Part of this effort to target new areas for acquisition has been aided by the use of GIS. With GIS the ownership layer overlain with the hydrography layer and the riparian layer will target new areas of interest. Sediment resulting from current and past overuse of rangeland also impacts the flowing streams and is the result of erosion within the upper segments of the watershed. The U.S. Forest Service using GIS is reviewing grazing allotment plans to determine if best management practices are being used within impacted areas. Locally along Oak Creek, a tributary to the Verde, subsurface discharges from septic tanks have caused concern. Sampling locations for water quality assessment were spotted; the alluvial aquifer was delineated; and restrictions were imposed for locating septic tanks within a specific distance from the streambank.

Grazing Best Management Practices

Our ultimate goal for grazing best management practices is to develop a system to evaluate BMP effectiveness in protecting water quality. The Department is developing a project whereby one can evaluate range utilization as a function of distance to water and other spatial attributes. Research has produced various models for the analysis of environmental components and for the prediction of systematic fluctuations in watersheds. Such models have been used to analyze the effect of environmental and cultural variations on systematic inputs, outputs, and processes. Frequently, increases in runoff and subsequent soil erosion have resulted in the sedimentation and organic contamination of surface waters. Increases in runoff are primarily the result of fluctuations in vegetation, soils, and climate. These fluctuations are a manifestation of the interrelated operation of natural hydrologic systems. The thesis is that grazing impacts to water quality can be evaluated as a function of continuous spatial attributes such as:

Precipitation;
Soil Type;
Distance to water; and
Pasture management techniques

Thus one will be able to compare erosion rates under different management alternatives.

FUTURE PROJECTS

Cumulative Hydrologic Impact Assessments

One frustration that I had when I started with the Department was the availability of data in relation to the activity proposed to be permitted. One had to go to at least ten different locations just to determine if there was any water to be concerned with in writing a permit. Then there was the case where an operation was being regulated by at least six different portions of the Department yet no one knew that there was any other interest by the Department in this operation. Furthermore no attempt was being made to evaluate the cumulative effects of multiple operations. Hopefully in the next few years permitting will be streamlined by the use of a GIS system.

In addition to permit evaluation, GIS could be used in the cumulative assessment and advanced identification of wetlands. Trends of wetland loss in a watershed over time could be studied and assessments made of the impacts of such losses.

Prioritization

The next major project will be a prioritization procedure to use our spatial data base to rank watersheds based on their pollution potential. By using GIS to prioritize, limited resources can be applied to the most critical watersheds.

The first stage of the prioritization method consists of identifying certain processes that have an effect on water quality. These can be ranked by color from light to dark within each category on a geographical basis. These processes may include: natural water quality, least impacted to most impacted water quality, amount of precipitation, ephemeral/perennial water flows, high precipitation to low, least erodible soil to most erodible, existing riparian areas to lack thereof, steep slopes to gentle gradients, and of most importance, the degree of use by man. When these are superimposed, the highest priority watersheds are revealed as light toned areas (McHarg, 1971).

Because nonpoint source pollution is often directly related to stormwater events, methods to determine the amount of flow and the constituents entrained in the flow are the most applicable. Prediction of the erosion potential of a specific area has always been a need of public and private land managers. Equations which assess erosion have proved to be very powerful management tools. The Universal Soil Loss Equation (USLE) is the best known and the most widely used of these equations. Several programs based on the USLE are available which can be used with the attributes stored in a GIS. Models being considered include AGNPS, SPUR, CREAMS, VirGIS, and WEPPs. The AGNPS model predicts erosion using grid cell information; SPUR is better for rangeland impacts; and the State of Virginia has an integrated

program called VirGIS (Hession 1988). The USLE has served us well; however, a better method is under development, the Water Erosion Prediction Project (WEPP). The USDA Agricultural Research Service (ARS) developed this model to replace the USLE for the use of the Soil Conservation Service, U.S. Bureau of Land Management and U.S. Forest Service. The model considers the effects of the major factors of climate, soil, topography, and land use on erosion. The WEPP model will apply to a broad range of land management practices. Evaluation of grazing effects, a variety of mechanical practices, disturbed forested areas, construction sites, urban and recreational areas will be possible. The model is intended to compute sheet and rill erosion where overland flow occurs. It will also compute erosion by concentrated flow in "ephemeral" gullies. Three versions are under development: the hillslope, the watershed and the grid versions. The Grid version will calculate erosion at all points and along all flow paths (at the grid resolution) within the area. (Windgate 1989) Pollution potential will be calculated based on the use of available models.

CONCLUSION

In conclusion, the power of a geographic information system is to be able to retrieve data based on its location and to be able to manipulate the data in relation to spatial orientations. The GIS system is cost-effective in comparison with manual procedures. Furthermore previously undetected relationships in data assist in the proper management of water quality in our environment.

Although the GIS system has been successful to date, three major constraints are seen as impacting future GIS work:

(1)   Time/staff training;

(2)   Obtaining equipment; and

(3)   Accuracy of data needed at the scale for a particular project.

The computer approach used by the Arizona Department of Environmental Quality in the Nonpoint Source Program has developed into a much larger, more useful system for the entire Department than anyone could have predicted. Work with other agencies has been key to any success that we have achieved.

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MARYLAND'S CHESAPEAKE BAY WATER QUALITY MONITORING PROGRAM: AN ESTUARINE WATER QUALITY INFORMATION SYSTEM

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INTRODUCTION

PROBLEM SETTING

The Chesapeake Bay and its tributaries have long been a valuable resource in terms of seafood harvest, shipping and recreation. These features, along with the fertile soils of the surrounding watershed, attracted some of the Nation's earliest European settlers. In the three centuries since then, population growth has been rapid. This growth will continue, resulting in an additional 20% population increase between 1988 and 2020 (2020 Panel 1988).

As in many other areas, population growth has led to serious pollution problems. The most prevalent and clearly identified threat to the Chesapeake Bay is eutrophication and its resultant impacts. Declining water quality due to eutrophication has been widely implicated in the concomitant decline of harvestable fish and shellfish although the relationship has never been quantified. Nevertheless, there is some evidence which suggests that habitat loss through lowered oxygen levels, sedimentation impacts on shellfish beds, decimation of macrophyte communities and possibly acidification of critical spawning sites have all contributed to the observed declines in living resources. Undoubtedly, overharvesting of fish and shellfish has contributed to their decline, but again the magnitude of this impact remains poorly understood to this day.

Potentially toxic metal and organic compounds have also entered the Bay and relatively high concentrations appear in the water, sediments and biota near industrialized locations such as Baltimore Harbor and the Norfolk area (EPA 1983). Little evidence exists, however, linking toxicants to harmful effects on the biota of the Chesapeake Bay. Human health concerns have been raised in some areas because of high tissue levels of some metal and organic contaminants in edible species. Increased attention is now being focused on achieving a better understanding of these potential toxicant threats in the Bay.

MANAGEMENT SETTING

Recognition of the problems caused by man first occurred in localized areas of the Bay where activities or populations were most concentrated. One clear example is the depletion of oysters in areas of concentrated harvesting activity which was noted in the late 1800's (Radoff 1971). Early recognition of water quality problems is best exemplified in the upper Potomac Estuary where raw sewage from Washington D. C. fouled the water by the late 1800's. Odors, algal blooms and bacterial contamination severely limited the river's use until recent years.

Environmental issues in general, and management of water pollution problems in particular, achieved national recognition with the establishment of the United States Environmental Protection Agency (EPA) in 1970 and the passage of the Clean Water Act in 1972. These actions enabled clean-up efforts in the Chesapeake Bay. In 1977 a 5-year study of the Bay was launched by the EPA. The findings of this study, released in 1983, led to a recognition of the Bay's problems on a much larger scale than

previously acknowledged. It drew attention to the intimate linkage between the Bay's mainstem, its tributaries and its 64,000 square mile watershed.

Since the EPA study, the states of the Chesapeake Bay region and several federal agencies have committed to work together in alleviating the Bay's problems. These commitments culminated in the 1984 and 1987 Chesapeake Bay Agreements signed by the governor's of Maryland, Virginia and Pennsylvania, the mayor of Washington D. C., and federal agency representatives.

ROLE OF THE MONITORING PROGRAM

One of the major conclusions from the EPA study of the Chesapeake Bay was that a comprehensive, long-term water quality monitoring program was needed to guide and provide accountability for management actions aimed at restoring the Bay's health. Since long-term Bay-wide water quality information was not available at the time of the EPA study, scientists trying to evaluate the Bay's condition were severely hampered in quantifying the extent and character of its problems. This piecemeal information was also of little value in defining the changes in water quality between the 1950's and 1970's as pollution entering the Bay during that period increased. Given the large uncertainty, both then and now, in our understanding of the Bay's ecological relationships, a comprehensive long-term water quality monitoring program was seen as a way of providing a "bottom-line" answer to the questions about man's impact on the Bay and its response to pollution control actions.

Uncertainties surrounding the quantification of pollution sources, their impact on water quality and, in turn, the impact of water quality on fisheries limit effective remedial action. Fortunately, Maryland and other jurisdictions have not let this uncertainty paralyze their efforts to reduce pollution entering the Bay. Given some of the obvious pollution problems of the last several decades such as raw sewage, odors, fish kills, bacterial contamination, and massive algal blooms, it was clear that certain measures such as secondary treatment and disinfection at sewage
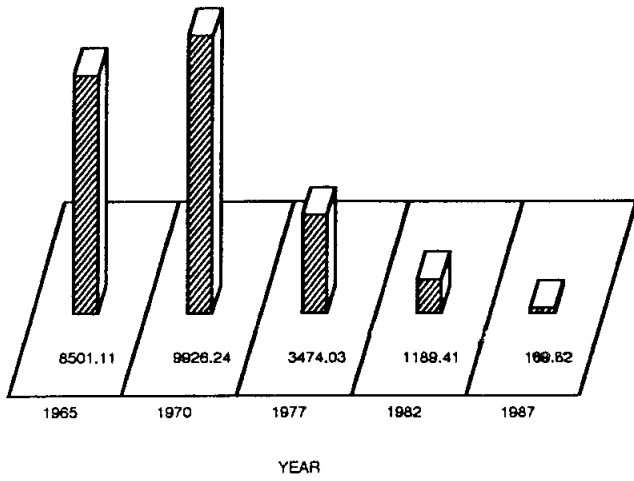
treatment plants were necessary. In recent years, more sophisticated analyses using mathematical models have provided justification for more concerted action in heavily polluted tributaries. As many of these remedies have been implemented, some dramatic improvements have been noticed (Fig. 1).

Today, however, the effects of eutrophication are more subtle and widespread. Oxygen concentrations often drop to levels that will not support fish and shellfish. Reduced water clarity and nutrient enrichment have made it difficult for macrophyte communities, which provide important habitat, to flourish as they had in the past. The Bay's bottom sediments have been altered so that in many areas they no longer serve as suitable habitat for the once abundant oyster. The sediments can also magnify external nutrient inputs by recycling back into the water column a large part of the nutrients that are deposited to the bottom.
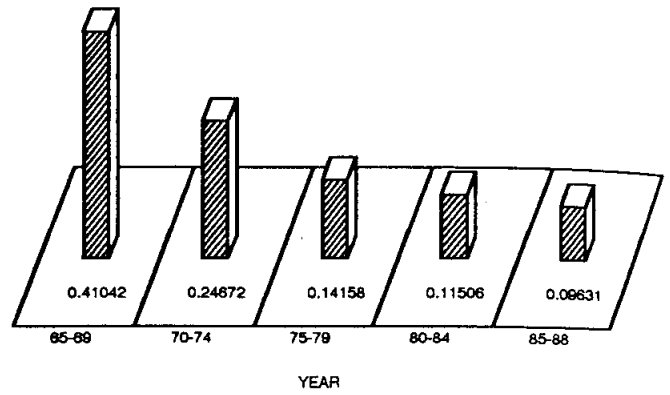
These continuing problems will clearly be more difficult and expensive to fix, especially in the face of increasing population pressures. Costly methods of advanced treatment at municipal and industrial plants are generally required now to make additional reductions in nutrient inputs from point sources. At the same time that nutrient removal is becoming more costly, the federal government is reducing support for these pollution controls. Nonpoint sources of pollution are starting to be addressed by more aggressive agricultural and urban programs but their effectiveness in stemming nutrient inputs to the estuary is poorly understood.

Given the level of uncertainty regarding the Bay's response to pollution and the increasing cost of pollution controls, there is a danger of pollution control programs losing momentum in the near future. We believe that the resolve of politicians and the commitment of citizens to spend the necessary funds for pollution controls are directly related to the value of the resource being protected and the confidence that pollution abatement programs will succeed (Fig. 2). The tremendous commercial, recreational and aesthetic value of the Bay is rarely questioned by the politicians
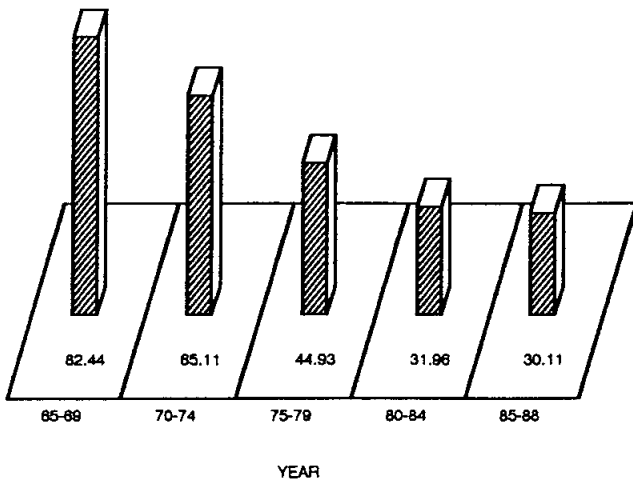
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Phosphorus Loadings From Sewage Treatment Plants

8501.11 9926.24 3474.03 1189.41 169.62

1965 1970 1977 1982 1987

YEAR

Phosphorus Concentrations In Water Column

0.41042 0.24672 0.14158 0.11506 0.09631

65-69 70-74 75-79 80-84 85-88

YEAR

Chlorophyll Concentrations In Water Column

82.44 65.11 44.93 31.96 30.11

65-69 70-74 75-79 80-84 85-88

YEAR

Dissolved Oxygen Concentrations In Water Column

3.9 3.3 5 5.8 6

65-69 70-74 75-79 80-84 85-88

YEAR
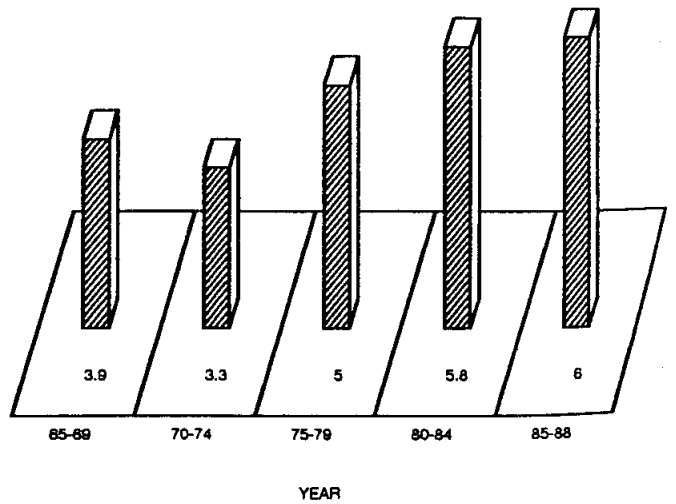
Fig. 1. Progress in reducing phosphorus loadings and resultant improvements in water quality in the tidal fresh portion of the Potomac River.
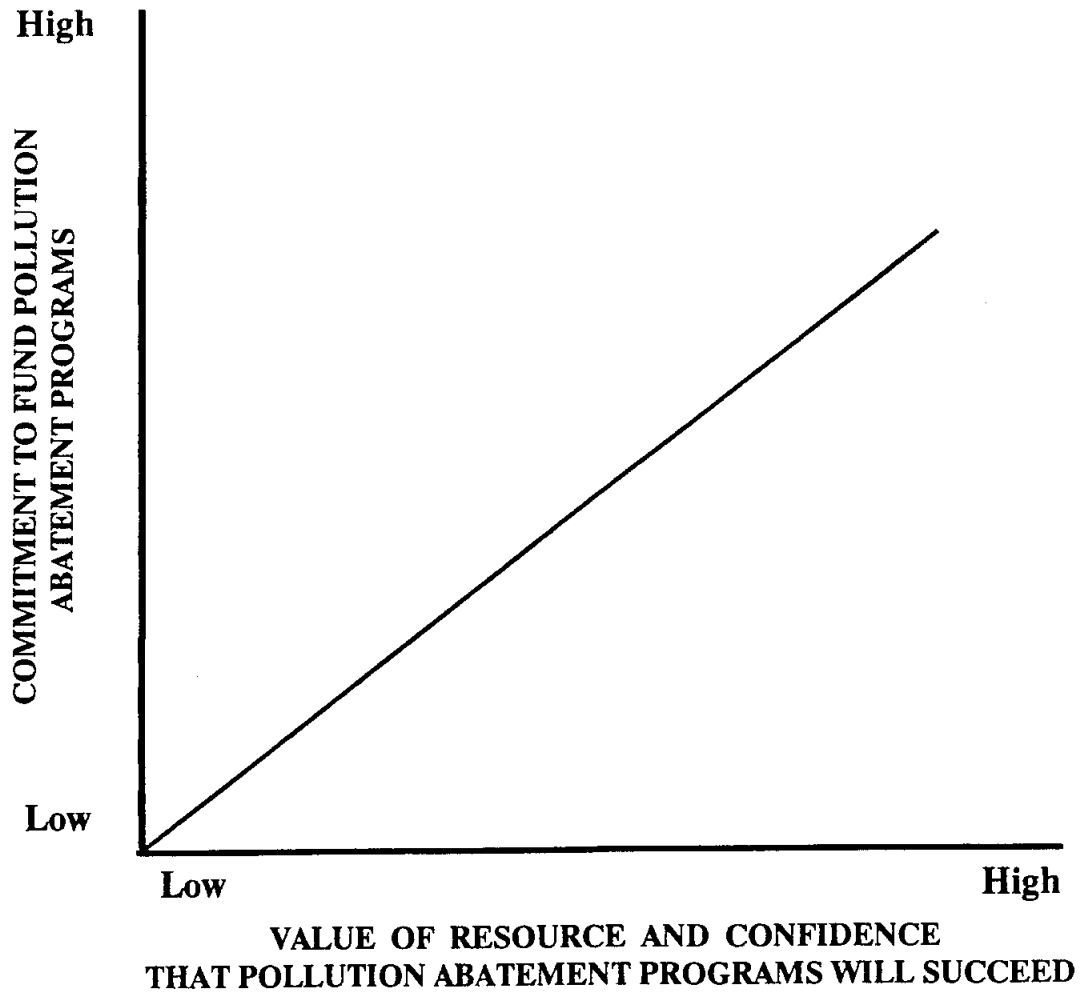
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Fig. 2. Realtionship between commitment to fund pollution abatement programs and both the value of the resource being protected and the confidence that pollution abatement programs will succeed.

or citizens of Maryland. Confidence in the precise direction of pollution abatement programs is not so high.

The Chesapeake Bay Water Quality Monitoring Program that Maryland implemented in 1984 is specifically aimed at reducing current levels of uncertainty in pollution abatement strategies. Along with other evaluations, such as forecasting the outcome of alternative strategies using mathematical models, the monitoring program provides information sufficient to justify needed management actions. Concepts that went into the program design and the ways in which the information is being used will be examined more closely in the following sections.

PROGRAM DESIGN

"CLOSING THE LOOP" BETWEEN WATER QUALITY ISSUES AND MANAGEMENT ACTION

Maryland's Chesapeake Bay Water Quality Monitoring Program is intended to serve a key role in directing and evaluating management actions aimed at improving water quality. In order to effectively achieve this overall objective, it was recognized that an unbroken sequence of events was needed from the identification of water quality issues through various phases of the monitoring program and ultimately to implementing management actions that would alleviate the identified water quality concerns. This sequence of events is depicted in Fig. 3. Many of the steps used in developing Maryland's monitoring program are similar to those identified by others (e.g. Ward and Loftis 1989) although here the circular arrangement of these steps further emphasize the ultimate use of the monitoring information. The sequence starts with the identification of water quality issues of concern. The next step in the process is to clearly define the monitoring information required by management. This information is then used to formulate a monitoring design and the program is implemented. After a period of time, information sufficient to play a useful role in water quality management is compiled. These results need to be rigorously analyzed and interpreted in the context of

directing or evaluating water quality management. Finally, the monitoring information, along with other relevant scientific, technological and economic considerations, is used to develop or modify a management strategy which then results in a specific management action. This use of the monitoring data (the final steps in the sequence) will occur a number of times during the course of a long-term monitoring program as new information becomes available and new management actions require evaluation.

By completing this sequence of events, the "loop is closed" between the water quality issues that initiated the monitoring program and the management actions that are taken to address these same water quality concerns. It takes a concerted, long-term commitment to close this loop and a failure at any one step along the way can block the utility of the monitoring program for management purposes. It is within this overall management context that Maryland's Chesapeake Bay Monitoring Program was formulated.

WATER QUALITY ISSUES AND MANAGEMENT INFORMATION NEEDS

To ensure that the monitoring program would ultimately be useful for management, its design was founded upon an assessment of information needs. This assessment commenced by defining the major water quality issues of concern. These were nutrient enrichment and its consequences: algal blooms, low dissolved oxygen and high turbidity. With observed declines in fish and shellfish abundance, these water quality concerns were strongly related to impacts on these organisms, either directly or through habitat deterioration. Toxicants were also a major concern, but there was much more uncertainty surrounding the effects of toxicants in the Bay and the information that would be useful for management purposes.

Starting with these broad management issues, more defined information needs were developed. This definition was facilitated by the listing of "management questions". These questions represented specific, practical pieces
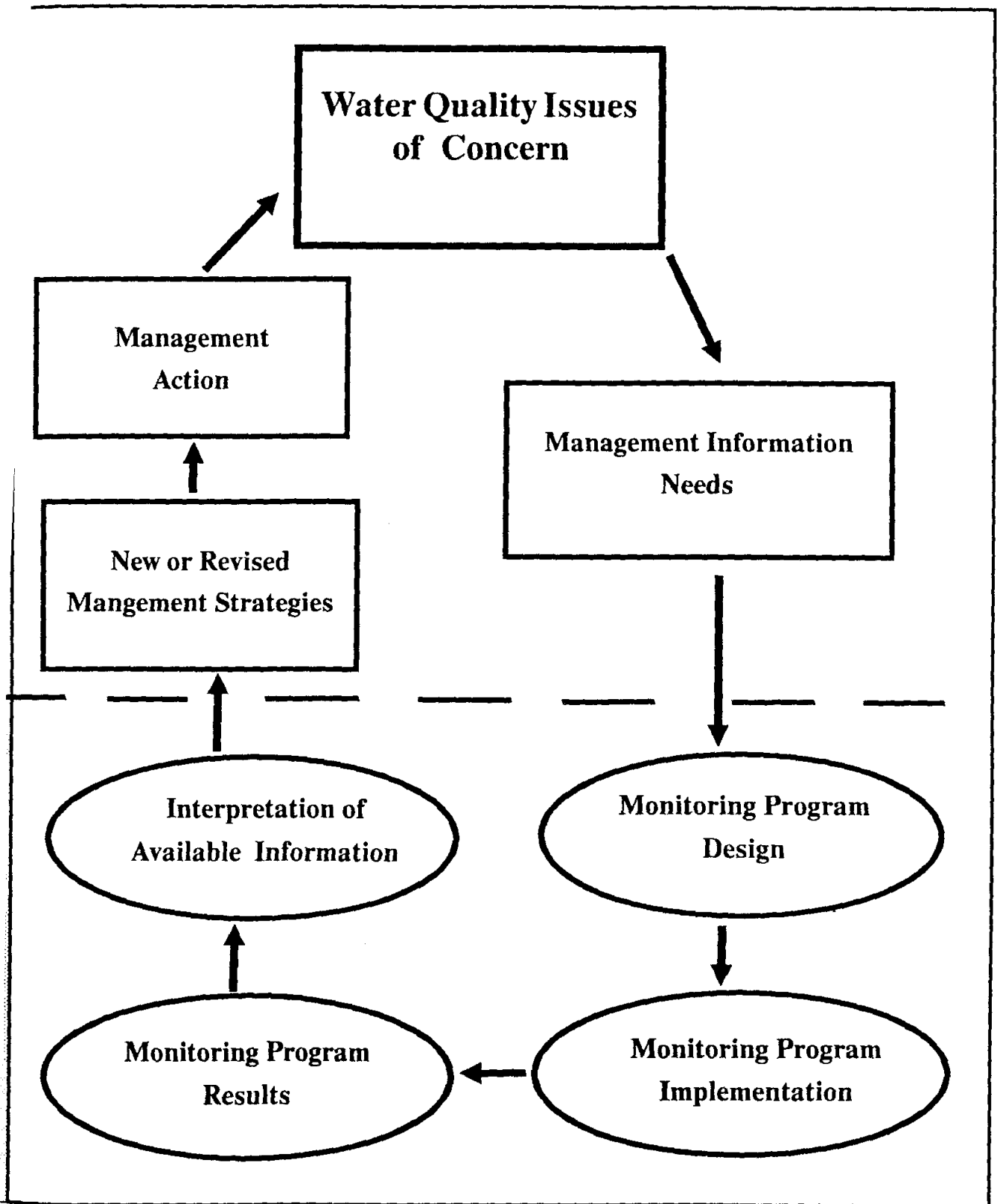
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Fig. 3. Sequence of steps linking management and monitoring. A monitoring program's goal is achieved when the "loop is closed" between the water quality issues that led to the development of the monitoring program and the resultant management actions that address these issues.

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of information that managers would need from a monitoring program to effectively pursue the restoration of the Chesapeake Bay. These questions requested information such as:

o What are the loadings of phosphorus and nitrogen from point and nonpoint sources in a particular basin?

o Where are hypoxic areas located and how severe are they?

o Has water quality improved where major management actions have been implemented?

o Is algal production limited by nitrogen, phosphorus or both?

From a long list of specific questions, or management information needs, three categories clearly emerged:

1. Questions about the present characteristics of water quality and pollutant loadings.

2. Questions about trends or changes in water quality due to increasing or decreasing pollution.

3. Questions about basic processes affecting water quality and the impact on fish and shellfish.

These information categories, then, became the three guiding objectives for the collection of monitoring information:

1. CHARACTERIZATION: Quantify the extent and nature of water quality problems.

2. DETECTION OF CHANGES OR TRENDS: Determine the response of key water quality variables to management action or inaction.

3. UNDERSTANDING OF PROCESSES: Develop and test hypotheses on how the Bay ecosystem functions, especially as it relates to anthropogenic stresses and management solutions.

Some additional themes also emerged from the long list of monitoring information needs. First, several types of water quality information would be required. Water quality is a general term and from a eutrophication standpoint it was clear that key physical, chemical and biological indicators were all needed to make informed management decisions. Second, the information needed to be collected Bay-wide in the mainstem and in each of the major Bay tributaries. This would provide data sufficient for decisions that reflect the Bay-wide nature of many problems as well as tributary-specific characteristics and solutions. Finally, the information needed to be collected consistently over a long period of time. Only with this long-term record could the monitoring program be effective in judging the success of management actions.

PROGRAM COMPONENTS

With specific information needs and objectives established, the design of the program could be formulated. From an assessment of the types of information that would be critical to management, six program components were formed. These were:

1. CHEMICAL/PHYSICALPROPERTIES
Variables: salinity, temperature, Secchi depth, dissolved oxygen, suspended solids, nutrient species (N, P, C and Si), phytoplankton pigments, heavy metal and organic compounds in surficial sediments.

Stations/Yearly Sampling Frequency: 77/12-20 (sediments, 1)

2. PHYTOPLANKTON
Variables: species counts, phytoplankton pigments by horizontal and vertical in vivo fluorescence, primary productivity, light penetration.

Stations/Yearly Sampling Frequency: 14/18

3. ZOOPLANKTON
Variables: micro (44um - 202um) and meso (>202um) species counts, biomass. Stations/Yearly Sampling Frequency: 14/12

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4. BENTHIC ORGANISMS
Variables: species counts, production, sediment characteristics, salinity, dissolved oxygen.

Stations/Yearly Sampling Frequency: 31/10

5. ECOSYSTEM PROCESSES
Variables: sediment-water column exchange rates of dissolved inorganic nutrients (N, P, Si) and oxygen; surficial sediment characteristics; deposition rates of particulate matter (total seston, N, P, C, phytoplankton pigments).

Stations/Yearly Sampling Frequency: 10/4 (exchange); 1 / 20 (deposition).

6. RIVER INPUTS
Variables: flow, suspended solids, nutrient species (N, P, C and Si), phytoplankton pigments.

Stations/Yearly Sampling Frequency: 4/20-30 (flow-dependant).

Station locations for most of these elements are displayed in Figure 4.

Each program component was structured such that it would provide both sufficient information for that discipline and complement others. It was recognized that these program divisions were somewhat artificial in the context of a complex, interacting ecosystem but that they were necessary to effectively design and manage such a large project. Knowing at the outset that the information would need to be interpreted across components, close linkages were created between most of the components by overlapping station locations and simultaneous sampling. This is particularly evident between the chemical/physical, phytoplankton and zooplankton components which are sampled from the same vessels. In this case, there are compelling scientific reasons for simultaneous sampling as well as the obvious resource efficiencies.

It was not feasible to implement all of the monitoring components in all of the Bay's tributaries. The chemical/physical component was conducted at the full complement of stations in the mainstem and tributaries. This component includes the most fundamental and interpretable water quality variables for management information needs. To provide a level of effort capable of yielding technically rigorous information, the other components were concentrated in the Bay's mainstem and Maryland's three largest tributaries. Baltimore Harbor was also included in most of the components due to its high pollutant impacts. By concentrating effort in the largest systems of the Bay, the broader water quality responses to management actions and an improved understanding of processes could be firmly established for these systems. This fundamental understanding, along with direct measures of chemical/physical properties, could then be utilized in the management of smaller systems. Variable selection, sampling methodology and spatial/temporal intensity were carefully evaluated for all components to provide a level of information that would be the minimum necessary to support confident management decisionmaking. Techniques such as statistical power analysis and pilot studies were used to evaluate study design where the literature did not provide sufficient guidance.

DATA MANAGEMENT

For a program of this magnitude and with little established precedent, data management was one of the most difficult hurdles to overcome. The requirements of the data management system were that it:

o create computerized data sets of all variables with rapid (2-6 mo. from sampling) turnaround;
o consist of formats that were readily accessible for data analysis;
o contain few errors;
o contain adequate documentation;
o provide flexibility for changes;

The entire system - data sheets, keypunching specifications, file structures, extensive programming to automate most aspects of data management, documentation standards, quality assurance, etc. - had to be newly created. It took over 2 years to reach a level at which the performance of the data
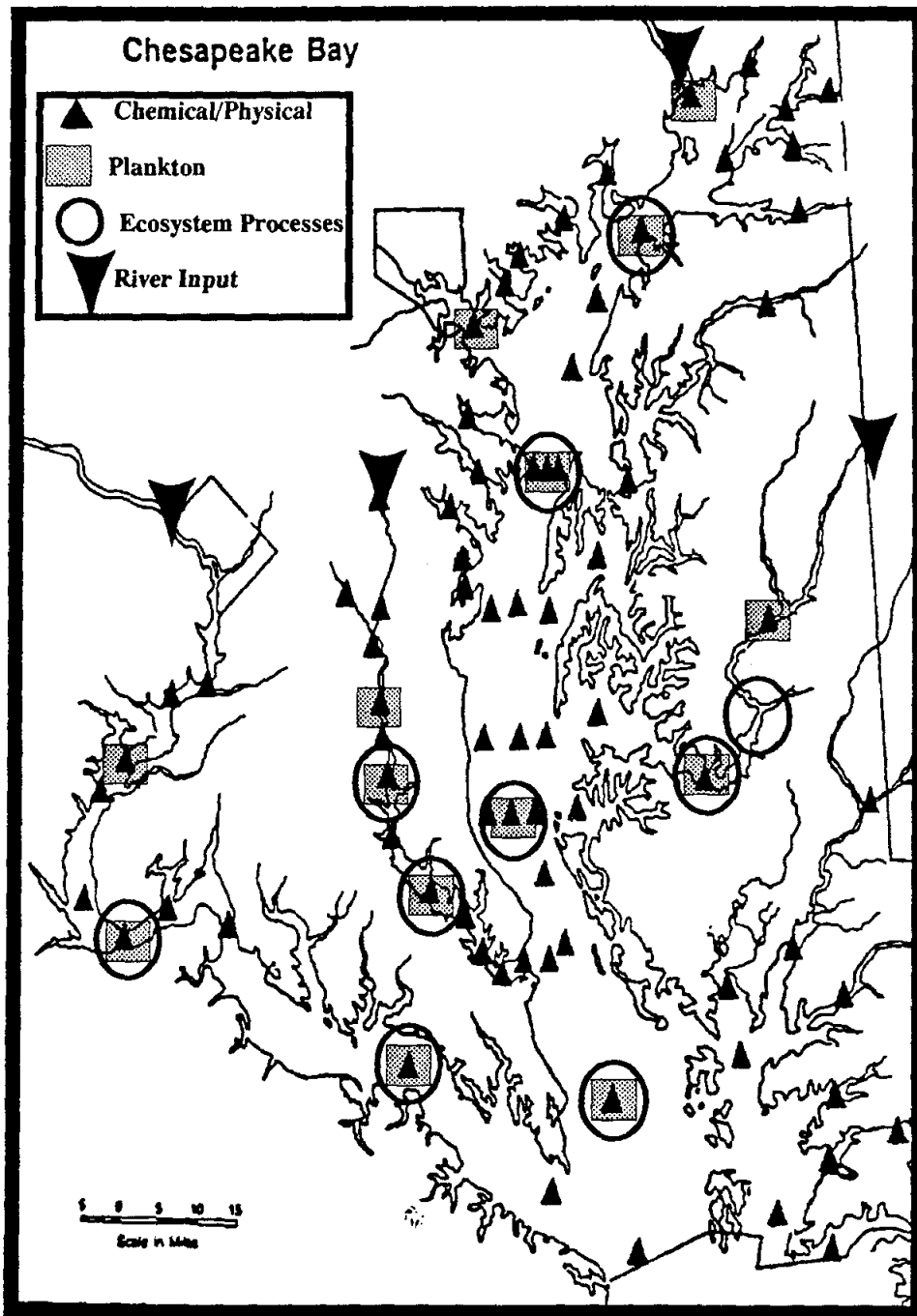
Fig. 4. Map of stations for chemical physical properties (▲),
phytoplankton and zooplankton (▨) and ecosystem processes(○).
Benthic organisms are sampled at 28 stations in the mainstem and major
tributaries.

management system was sufficient to support all of the requirements listed above.

DATA ANALYSIS AND REPORTING

The element of the monitoring program that finally brings the information into the management arena is data analysis and interpretation. Maryland's strategy includes both technical and non-technical summaries of the monitoring information and reflects the input of other sources of information into the decisionmaking process. While competent technical analysis is the foundation for utilizing the monitoring information in management decisions, a parallel effort is being made to inform politicians and citizens. The politicians and citizens are viewed as being an important part of the water quality management decision process. They supported the creation of the monitoring program and expect it to provide periodic reports on the "State of the Bay" as well as serving water quality managers in the regulatory agencies. Ultimately, it will be the citizens of Maryland and their elected officials that decide the allocation of resources to restore the Bay.

Information from the various sampling programs is transferred to computerized data formats as described in the previous section. The first level of technical reporting for the program is termed the "Level I Report". These reports summarize and interpret the information for each of the individual monitoring components and are updated annually. They contain cumulative information from the inception of the program and, where available, historical information collected before this program started. These reports serve to fulfill the first two objectives of the monitoring program - characterization and detection of trends or changes - for each individual component. They also serve as a readily accessible form of information to facilitate the assembly of a "Technical Synthesis" among the various disciplines.

The "Technical Synthesis Report" is where the different components of the monitoring program are brought together for multi-disciplinary analysis of the water quality issues that the program was developed to address.

Here, the characterization and trend/change detection objectives are evaluated from a broader water quality perspective. And, in the Technical Synthesis, the third objective of the program - understanding of processes - is addressed. In satisfying this third objective, relevant research and mathematical model findings are incorporated into the analysis of monitoring information. The next step in preparing the monitoring information is to condense the detailed technical findings into the most relevant information for management purposes.

In making the monitoring information useful for Bay management, two final paths are taken. One provides distilled technical findings and recommendations to water quality managers in the Maryland Department of the Environment and other state and federal agencies cooperating in the Bay restoration. The other provides summarized non-technical information to Maryland's citizens and politicians. The information is presented both as regular comprehensive reports addressing the Bay-wide scale and as tailored interpretations for issues of more limited scope. Examples of the distilled technical findings range from a comprehensive Bay-wide treatment of the information which is planned for 1991 (1991 Re-Evaluation of Nutrient Reduction Strategies) to more limited scopes which include decisions at individual sewage treatment plants and assessments of localized water quality problems. The program's biennial legislative summary, "Monitoring for Management Actions" (Magnien et al 1987), is an example of a comprehensive non-technical document which provides legislators and citizens with a status of Chesapeake Bay water quality and an update on the progress of the clean-up efforts.

PROGRESS TO DATE

In the summer of 1984, following a year of planning, the monitoring program described above was implemented. With 5 years of monitoring information to date, the program has largely achieved its first objective of establishing an initial Bay-wide character-ization of water quality. In some tributary estuaries, such as the Potomac and Patuxent Rivers, clear changes in water quality have

been established in response to nutrient loading reductions. In the case of the Potomac River, various monitoring programs had been in operation since the 1960's. These data were combined with the more recent monitoring data to establish trends over an extended period of time (see Fig. 1). The Potomac River monitoring information clearly demonstrates that a monitoring program of the type now in place can provide definitive, quantitative answers on the response of an estuarine system to concerted management efforts. This capability fulfills the second major objective of the Maryland program.

Considerable progress has also been achieved on the third objective of the monitoring program, an improved understanding of processes related to water quality in Chesapeake Bay. A much clearer picture is emerging from analysis of the monitoring data on such key eutrophication issues such as the sources and fates of nutrients, the spatial and temporal patterns of limiting nutrients and the current utilization pathways for primary production. This information is now being assembled into the previously described "Technical Synthesis" that will include a rigorous analysis of the first 5 years of monitoring information. These results will be used in refining both mathematical and conceptual models which are being used to predict the response of the Bay to various management strategies.

Although the monitoring program has been quite successful in meeting its design objectives, the most important measure of its success is whether or not the monitoring information has been used in the management of Chesapeake Bay. Already, there are a number of examples where it has been used. The first two years of monitoring data were used in the development of a 2 - dimensional mathematical model of the Bay. The nutrient reduction scenarios of this model led to the most dramatic commitment of the 1987 Bay Agreement - a 40% reduction of nitrogen and phosphorus by the year 2000. This agreement, signed by the Governors of Maryland, Virginia and Pennsylvania, the mayor of Washington D. C., and top federal agency officials has resulted in specific nutrient control actions. Similarly, a thorough analysis of monitoring

data and the use of monitoring data for the development of a mathematical model was the foundation of a decision by EPA to grant Maryland $10 million to remove nitrogen from a major sewage treatment plant on the Patuxent River. The monitoring information has also supported management in more subtle ways. By actual demonstration of positive responses to management actions in the Potomac and Patuxent Rivers, the monitoring information has greatly enhanced the confidence among managers that nutrient loadings reductions will produce desired results in the estuary.

FUTURE CHALLENGES AND DIRECTIONS

Many additional challenges confront the monitoring program as the Bay's future restoration plans are periodically reformulated and assessments are conducted on the results of previous efforts. The 1987 Bay Agreement commits to a "re-evaluation" of the goal to reduce nutrients by 40%. Interpretation of the monitoring information, both directly and through the use of improved mathematical models, will be the technical cornerstone for this re-evaluation. Because monitoring is now being conducted in most of the Bay's tributaries, the re-evaluation will provide an opportunity to improve upon strategies in many areas by resolving future plans on a basin-specific level. Analysis of the monitoring information to date has provided strong justification for the basin-specific approach for nutrient reduction since large differences exist between many of the tributary and mainstem regions in terms of the concentrations of nutrients in their waters and the sources and amounts of nutrient loadings.

Another question that relates strongly to the monitoring programs is the concept of goal setting for water quality. In grossly polluted situations it is clear that desirable water quality conditions are not being met. As pollution reduction programs eliminate many of these obvious problems, the question turns to how "good" does the water quality need to be. As logical as it seems to have a goal when considerable resources are allocated to mitigate a problem, the desired water quality - or goal - remains poorly defined.

One definition of a water quality goal - that which protects human health - has received the most attention and at least some guidelines exist regarding bacterial contamination. Goals related to the eutrophication problem in estuaries have not received much attention except for dissolved oxygen. Levels below 4 or 5 mg/l are typically considered a stressful condition for fish and shellfish. In stratified estuaries such as the Chesapeake Bay, however, application of these guidelines is difficult since naturally occurring dissolved oxygen levels are often below these thresholds.

The current focus for setting goals is the relationship between water quality conditions and the Bay's living resources. There is a widely-accepted perception that deteriorating water quality has contributed to many of the fish and shellfish declines in Chesapeake Bay. Efforts are underway to identify the minimum water quality conditions that are necessary to support the successful reproduction and survival of fish and shellfish. Monitoring information is being used both in the development of these goals and in their application in the estuary. While many of the initial criteria for water quality conditions may come from controlled laboratory experiments, they need to be tested by evaluating monitoring data on the coincident distributions of the organisms in question and the existing water quality. Once firm numbers are established, the monitoring data can then be used to identify areas where conditions are not suitable for certain species and that may be a priority for pollution abatement actions.

A continuing challenge for the future will be to build upon the cooperative nature of current efforts to restore the Bay. Recent Chesapeake Bay agreements have brought together state and federal agencies in an unprecedented regional approach to solving the Bay's problems. These agreements have committed to a coordination of programs from the highest levels of government to the levels at which programs such as water quality monitoring are conducted. Many of the current monitoring programs have been established or fine-tuned under this cooperative umbrella. It is now possible to evaluate nutrient inputs from the Pennsylvania, Maryland and Virginia watersheds as well as to examine water quality conditions throughout the Maryland and Virginia portions of Chesapeake Bay. With the firm technical underpinnings that the monitoring programs provide, these cooperative efforts to improve conditions in the Bay serve as a model for other estuaries around the country.

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SOIL AND WATER QUALITY MONITORING PROGRAMS

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ABSTRACT

Standard procedures for the design of environmental monitoring projects have been developed for government facilities that are operated by Rockwell International in Colorado and California. The procedures provide guidance for identifying and quantifying information goals; establishing statistical design criteria; determining which variables to measure, and where and how frequently to sample; performing statistical testing and analysis; developing operating plans and procedures for sampling, chemical analysis, data analysis, data management and quality assurance; and establishing procedures to report information and to evaluate the performance of the monitoring system. The procedures provide a systematic approach to the design of monitoring programs and are intended to be used for regulatory compliance monitoring, routine environmental surveillance and special sampling projects. Application of the design procedures is illustrated with a monitoring plan developed to characterize background hydrogeochemistry at the Rocky Flats Plant in Colorado and to detect soil and water quality changes resulting from plant operations.

INTRODUCTION

Environmental monitoring programs have been established at industrial facilities throughout the world. However, many of these monitoring systems have been set up without specifying the goals and objectives of the program; the methods for data collection, storage, validation, and analysis; the information reporting procedures; when will enough information have been collected; and how the data will be used to make environmental management decisions.

In order to assist designers in identifying specific objectives and to design monitoring systems that provide the information necessary to meet the objectives, standard procedures for the design of environmental monitoring systems have been developed for government facilities that are operated by Rockwell International in Colorado and California (Greengard, 1988). The procedures, which are based on recommendations for water quality monitoring systems by Colorado State University researchers (e.g., Sanders et al ., 1983; Ward, 1985; Ward and Loftis, 1986), provide guidance for identifying and quantifying information goals, establishing statistical design criteria; determining which variables to measure, and where and how frequently to sample; developing operating plans and procedures for sampling, chemical analysis, data analysis, data management, quality assurance and personnel protection, and establishing procedures to report information and to evaluate the performance of the monitoring system. The procedures provide a systematic approach to the design of sampling plans and have been written for environmental monitoring programs in general, thus they should prove useful in developing plans for a variety of purposes, including routine environmental surveillance, special investigations, process emissions/ effluent monitoring, waste stream character-

ization, regulatory compliance, and remedial action monitoring.

The procedures, and this summary paper, have been organized according to the flow of information required to design a monitoring system. Thus, requirements for an evaluation of information expectations are presented first followed by statistical design and characterization, network design, operating plans and procedures, and information reporting and utilization. A case study is presented that illustrates the application of the design procedures.

INFORMATION EXPECTATIONS

The development of information expectations, i.e., the information that managers and users expect to receive from a monitoring system, involves determining environmental (e.g., water, soil, air) quality and problems, regulatory requirements, management goals, monitoring objectives, statistical design criteria, reporting requirements and information use. Environmental Problem Statement

A sampling plan should describe the environmental problems and concerns that led to the initiation of the monitoring project. The plan should provide information on specific environmental concerns, general history and project background, the current situation, the projected impact(s) to the environment if no action is taken, what the environmental goals are, and how the goals can be achieved. Defining goals and the method(s) of achieving those goals involve management decisions that can be derived from the problem statement. They must be converted to monitoring objectives as part of the design process.

Statutory and Regulatory Requirements

As regulatory information expectations are derived directly from the legal requirements, the first step should be to review the federal and state statutes. This step involves identifying what information expectations and monitoring requirements are stated or implied by the statutes and by the administrative/ regulatory agency's functions and powers.

These functions and powers are listed in the statute and serve as administrative tools to promote compliance with the law and its objectives. Examples of administrative functions and powers include permitting authority, promulgation of standards and criteria, and enforcement action. The administrative agency named in the law is responsible for setting policy, formulating specific regulations to meet the objectives set forth in the statute, and providing supplemental guidance documents to help regulated parties achieve compliance with the regulations. The regulations and guidance should be reviewed and a determination made as to whether or not the statutory objectives can be achieved through the monitoring prescribed by the administrative agency. It should also be determined whether all the technical requirements specified in the regulations are necessary to achieve the intent of the law. If not, comments can be submitted on proposed regulations or unnecessary requirements can be challenged through the legal process.

Management Goals

Management goals can be developed from the problem statement and legal/regulatory objectives and requirements for monitoring. A clear definition of goals is a prerequisite for monitoring because monitoring reports must demonstrate that the program has achieved, or is achieving, the program goals. Examples of management goals, some of which are derived directly from various laws, include "protect" the environment, "maintain or improve" environmental quality, "determine" air or water quality, "assess" environmental impacts, "comply" with regulatory permits or standards, "mitigate" adverse impacts, "evaluate" clean-up progress.

Monitoring Objectives

Once management goals have been defined, they must be converted into specific monitoring objectives. For instance, in order to achieve regulatory compliance (a management goal), compliance must be defined and the monitoring system must be able to measure compliance. Common monitoring objectives derived from

management goals are determining: 1) average conditions, e.g., measurement of central tendency (means or medians) at stations throughout a specified area; 2) changing conditions, e.g., measurement of trends at a station(s) over time; and 3) extreme conditions or regulatory compliance, e,g., exceeding a limit or permit condition or the probability of exceedance (violation). Since monitoring results must be able to demonstrate that management goals have been attained, management goals must be viewed in terms of possible monitoring results. For example, in order to attain the management goal of "restore and maintain", the numerical values of environmental quality parameters must decline to a baseline or predetermined level and then remain constant or continue to decrease.

Statistical Design Criteria

Once the problem has been defined, and management and monitoring goals identified, then the type of statistical approach to use to obtain the information must be evaluated. How the data will be analyzed and how the monitoring objective will be translated into a statistical hypothesis that can be tested must be determined. The statistical methodology, types of statistical results and plans to present the data and results must all be defined as part of the quantification of information expectations. The statistical approach should be related to the monitoring objectives and the monitoring objectives should be related to the management goals. This can be accomplished by establishing the information desired, the statistical methodology to produce the information from the data, the assumptions underlying the statistical approach, and the type of statistical conclusion that will result from using this method(s). Finally, whether that type of statistical conclusion (with its associated uncertainty) measures or supports the attainment of the management goal(s) must be assessed.

The amount of uncertainty that can be tolerated depends on the intended use of the data. The level of uncertainty that is acceptable is a critical part of the monitoring network design, i .e., what, where, and how

often to sample, and therefore must be incorporated into the statistical design criteria. The statistical design criteria should be regarded as a measure of performance for the monitoring program because they set limits on the confidence in the data by specifying the acceptable uncertainty in the estimated variables.

Information Reporting

The report should be the focus of the entire monitoring system. The report presents the information and should be designed to meet well-defined information expectations. Therefore, the report must be carefully tied into management and monitoring goals. The frequency, format, contents and anticipated uses of reports should be defined as part of the establishment of information expectations. The moni4oring reports should provide an evaluation and discussion as to whether or not the program goals and objectives have been attained.

STATISTICAL DESIGN AND CHARACTERIZATION

Statistical methods can be applied to both monitoring system design and data analysis. Statistical design consists of developing specific hypotheses, statistically characterizing the population to be measured and confirming that the statistical approach and specific methods selected to obtain the desired information do not have their underlying assumptions violated by the population characteristics (Ward and McBride, 1986).

Statistical Characterization and Testing

The selected statistical methods must match both the information expectations of users and the characteristics of the population to which they are applied. Therefore, available data must be analyzed to determine the statistical characteristics of the population being monitored. Then, the assumptions and requirements of proposed statistical tests must be compared with the characteristics of the population. As Loftis et al. (1986) point out, the results of the analyses are questionable when the assumptions of the statistical methods are violated. If data do not already

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exist, a set of data will have to be collected as part of a phased design approach. That set of data will provide the basis for detailed system design. The design process should always involve review and evaluation of design assumptions and design modifications as data are collected and analyzed.

For many environmental contaminants, the assumptions of independent, normally distributed data are not realistic because environmental data are commonly correlated and non-normally distributed, and the variance may change over time (Gilbert, 1987). For water quality data in particular, there are three assumptions which appear to be of most concern (Ward and Loftis, 1986; Loftis et al., 1986): 1) independence of observations including the absence of seasonality or serial dependence; 2) homogeneity of variance over the period of record; and 3) form of the probability distribution, e.g., normal or non-normal. Results of a recent review of ground water quality data indicate that many ground water quality variables are not normally distributed, but have skewed right distributions; can exhibit seasonal fluctuations of various shapes and magnitudes, especially in shallow or highly permeable aquifers; and can exhibit significant serial correlation when samples are collected quarterly (Montgomery, Loftis and Harris, 1987). For these reasons, the statistical characterization of environmental data should include time series plots and testing for normality, homogeneity of variance and independence.

As part of quantifying information expectations and establishing design criteria, statistical hypotheses should be developed from the overall monitoring goals and objectives. The specific hypotheses to be tested are identified and the statistical procedures for testing the hypotheses are selected as part of statistical design. For example, if a major goal is to identify trends in water quality, the trend can be measured by a variety of tests (Sanders et al., 1983), e.g., testing for a linear trend in the raw data, in the annual means, in water quality indices, in the residuals after seasonal variation and serial correlation effects have been removed, or testing for temporal changes in population characteristics. The choice of which test to

use depends on management goals and the anticipated decisions that may be made if a trend is, or is not, detected. The specific hypotheses and the alternative statistical methods for testing the hypotheses should be listed and summarized. Estimates of data needs for each test can then be developed and the level of confidence in test results can be evaluated relative to data needs (Sanders et al., 1983). At this point, the conflicts between available budget, staff resources and worth of information can be evaluated and resolved among management, information users and system designers.

Statistical Methods

A review of statistical methods is outside the scope of this paper. A more complete discussion is provided in the design procedures manual (Greengard, 1988) and in the following references which describe appropriate statistical methods for environmental data analysis including methodology, applicability, advantages and disadvantages. A review and synthesis of the role of statistical design criteria in monitoring system design, plus a summary of methods for testing normality, homogeneity of variance and independence, and methods of measuring central tendency, trends and extreme Yalue probabilities is provided in a paper by Ward and Loftis (1986). Gilbert (1987) presents a thorough discussion of the statistical approaches to the analysis of non-normally distributed data and outliers, and the use of control charts. Concepts of probability and statistics applicable to water quality monitoring are described in Sanders et al. (1983). A detailed discussion of general characteristics of ground water quality random variables and statistical methods for characterizing these variables and detecting changes in ground water quality has been prepared by Colorado State University (Loftis et al., 1986). Guidance in analyzing limited background data sets and selecting statistical methods to characterize ground water quality is provided by Harris, Loftis and Montgomery (1987). Statistical procedures to detect leaking at hazardous waste facilities are addressed by Doctor, Gilbert and Kinnison (1986) and by the U. S. Environmental Protection Agency (1988, 1989). Specific

applicability of the t-test as opposed to nonparametric methods for detecting trends in water quality variables is discussed by Loftis (1985), Montgomery and Loftis (1987, 1988), and Helsel and Hirsch (1988).

NETWORK DESIGN

The term "network" refers to the physical layout of the monitoring system. Both physical and statistical components, i .e., variables to measure, sampling locations and frequency of sampling, are specified during network design. Sampling sites are identified based on watershed and hydrogeologic characteristics and the project goals. The variables to be measured are derived from the applicable environmental regulations, site environmental problem(s), management goals, and any interdependence between variables (Ward, Loftis and McBride, 1986). The frequency of sampling and analysis depends on the requirements of the statistical tests. Budgetary and operational considerations will usually influence final design of the network.

Selection of Variables to Measure

The variables to measure are dependent on the objective(s) of the sampling program. Certain variables may be specified by the applicable environmental regulations while it may be also prudent to measure other variables that influence the environmental behavior of the required variables. Before a monitoring network can be adequately designed, the variables to be monitored should be selected so that their variation in time and space, and the different statistical behavior of different variables can be considered during design (Sanders et al., 1983). Statistical variation will affect the selection of variables to measure, the location of stations and the frequency of measurement.

Location of Monitoring Stations

Statistical sampling requires that samples be representative of the water, air or soil mass. Therefore, the locations of sampling stations must be carefully selected in order to obtain a representative sample. Sampling locations should be specified in the monitoring plan and the selection of each site

justified. For instance, criteria for locating sampling stations to collect data for environmental or health risk assessments should insure that enough samples are collected to establish background conditions, delineate the source, the extent and magnitude of contamination, actual or potential environmental pathways, the impact on susceptible populations and to support modeling requirements. On the other hand, the number of samples should be minimized so that only those samples "necessary and sufficient" to meet the objectives of the investigation are collected.

Frequency of Sampling

Monitoring data are collected in order to estimate a statistical parameter accurately enough to satisfy the information goals. Since it is a parameter's variability (and analytical uncertainty) that prevents its exact determination, variability must be considered in selecting the frequency of sampling, i.e., the more variation, the more samples will be necessary to obtain a reliable estimate (Sanders et al., 1983). The objective is to determine the number of samples that will result in the confidence intervals specified as acceptable. The information goals will influence the selection of both confidence level and confidence interval widths. The concept that network performance is prescribed by the statistical design criteria leads directly to the determination of sampling frequency because the level of confidence in an estimate is a function of sample size. Therefore, if a certain variance or estimated range of possible values (intervals) of the sample mean is desired, and the population variance is known or can be assumed, the required sample size to achieve a particular level of confidence can be calculated. An interval estimate provides an upper and lower limit on the estimate of the population mean along with an associated probability that the true mean will be contained within a randomly selected interval. The interval estimate is a measure of monitoring network performance because it imposes boundaries on the estimate. For a specified confidence level, a narrow interval implies a large sample size and/or low variability and thus a high degree of

confidence in the estimate. Conversely, if the interval is wide, it implies a small sample size and/or high variability and hence, a low(er) degree of confidence. The network designer can control system performance by specifying (increasing or decreasing) sample size. To narrow the interval, the confidence level could be reduced. However, a decrease in the level of confidence may not be acceptable to either the technical staff, management or the regulatory agencies. Thus, the network designer must balance the number of samples collected against the level of confidence that is adequate to meet the monitoring objectives. Various aspects of network design including selection of variables, location of stations, frequency of sampling and statistical techniques are described at length in Sanders et al. (1983) for water quality monitoring.

OPERATING PLANS AND PROCEDURES

Before a monitoring system can begin generating data, specific plans and operating procedures must be developed to direct and control system operations. Procedures must be defined in sufficient detail so that they can be performed by different people and still generate identical results (Ward, Loftis and McBride, 1986). No procedure or operational detail should be left open to interpretation by field or laboratory personnel. Unclear or non- specific procedures lead to the classic and all too common situation where data generated one day (or week, month, quarter or year) are not comparable with data generated another day. Thus, procedures must be clear and complete enough so that personnel will make as few decisions in the field or laboratory as possible. Unanticipated and undocumented decisions may influence the variance in the data. Although all procedures will change over time as better methods and technology are developed and approved, no unauthorized procedural modifications can be tolerated in a well-run monitoring program. An official design and procedures modification process should be specified in the monitoring system design plan. Any modifications in procedures, whether authorized or unauthorized, even if only performed once, should be documented and reported with the data for that reporting period.

Other aspects of day-to-day operation which must be addressed in standard operating procedures are personnel, facilities, and equipment. Facilities and equipment must meet the system specifications if accurate information is to be obtained. Equipment failures may cause gaps in the data record, crowded facilities may result in lost or missing data, and contaminated laboratories will cause incorrect measurements (Sanders et al ., 1983). Training of personnel who will operate the monitoring system is critical to a successful program. Personnel operating the system must be properly trained and understand what is required of them. Training requirements for field, laboratory and office staff should be specified in the quality assurance plan.

The purpose of developing standard operating plans and procedures is consistency of operations. The procedures, facilities and personnel training should be designed to eliminate or at least minimize data problems such as missing values, outliers, sampling and analytical errors, etc. The success of the monitoring program must be viewed in terms of the quality of information developed from the data rather than in terms of the numbers of samples collected and analyzed (Sanders et al ., 1983). Quality assurance/quality control should be considered an integral part of the monitoring system. An effective quality assurance program ensures that the procedures followed are documented at each step in the monitoring process and that corrective action is taken where problems are noted. Procedures to document incl ude pre-sampl ing preparation, sample collection, sampling records and chain of custody, sample preservation, sample handling and transport, sample receiving, laboratory methods, laboratory reporting, database system procedures, data analysis methods, data verification, quality assurance/quality control, and health and safety. Each round of sampling and analysis must be thoroughly planned and controlled including scheduling, site access and equipment to be used. For the Rocky Flats Environmental Restoration Program, standard operating procedures (SOPs) have been developed for monitoring operations. The SOPs are reviewed regularly and revised when appropriate. Complete

records of the original and revised procedures including dates of implementation are maintained.

INFORMATION REPORTING

The purpose of monitoring is to produce information, not just data. Thus, the monitoring reports should be designed to convey the information considered necessary and expected to demonstrate that program goals have been, or are being, achieved. The monitoring data and results of the statistical tests should be presented and interpreted within the context of the program goals and decisions that will or should be made based on the information acquired. If the information is not used to make environmental management decisions then the entire monitoring program should be re-evaluated as to its purpose and worth in the decision making process.

Reporting procedures will vary depending on the program's goals, strategy, users, management and budget. However, the lack of specific reporting procedures is a common failing of monitoring programs and should serve as a warning that data collection may have become an end in itself (Sanders et al., 1983). In general, there are two basic types of monitoring projects, routine and special. Routine, permanent-station monitoring reports, e.g., for RCRA (Resource Conservation and Recovery Act) ground water monitoring , are issued periodically. Each report interprets the most recent data in terms of current environmental quality and compares current data to past data, both at a station and between stations. These reports are generally used to determine whether changes have occurred, to document whether regulatory compliance is being achieved and to assess the effectiveness of management controls. Special investigations generally consist of a high density of sampling sites in a relatively small area, sampled at a high frequency over a short time period (Ward and McBride, 1986). Reports of special investigations, e.g., CERCLA (Comprehensive Environmental Response, Compensation and Liability Act) remedial investigations, typically consist of a single report issued at the end of a phase of the project and/or a comprehensive

report integrating all phases of the investigation. The reports provide information to meet well-defined objectives such as identifying the nature, extent and magnitude of contamination, environmental impacts or risks.

In summary, the system design and operating plans and procedures should be developed to meet program goals and objectives, but they should not be considered the "heart" of the system. It is the information developed from monitoring that should be the focus of the entire program.

APPLICATION OF PROCEDURES

The design procedures summarized in this paper have been used to develop a plan for the characterization and monitoring of background soil and water quality at the Rocky Flats Plant near Denver, Colorado. Components for nuclear weapons are manufactured at the facility, and radioactive and hazardous wastes are generated in the manufacturing process. Both storage and disposal of these wastes have occurred at the facility. Preliminary assessments under the Rocky Flats Environmental Restoration Program have identified some of the past waste sites as potential or actual sources of environmental contamination.

The collection of background data will assist in the evaluation of environmental degradation by determining naturally-occurring spatial and temporal variability of soil and water chemistry. Background data will be compared statistically with data from a downgradient site (waste storage or disposal unit) to determine whether a particular chemical concentration represents a release from the facility. The statistical approach used in the plan follows the recommendations of Doctor, Gilbert, and Kinnison (1986); Loftis et al. (1986); Loftis, Harris, and Montgomery (1987); Gilbert (1987); and EPA (1988) for establishing baseline monitoring and detection systems at hazardous waste facilities.

Program Goals and Objectives

The plan is designed to accomplish the following management goals:

1) Establish a monitoring program to characterize background soil, surface water, and ground-water chemistry;

2) Determine impacts from Plant operations on soil and water quality; and,

3) Establish statistically sound regulatory ground-water monitoring programs.

Specific objectives have been developed to achieve management goals. Monitoring objectives are to determine:

1) Average Conditions -- Characterize central tendencies and variability over time (water chemistry) and space (soil and water chemistry) at background and downgradient stations;

2) Facility Impacts -- Identify differences in soil and water chemistry between background and downgradient stations;

3) Changing Conditions -- Detect and measure water quality trends at monitoring stations over time.

4) Regulatory Compliance -- Determine whether a release has occurred from a particular unit and whether a regulatory limit or standard, i.e., CERCIA applicable or relevant and appropriate requirement (ARAR) or RCRA ground-water protection standard, is being exceeded at background or downgradient stations or RCRA compliance points.

Data Quality Objectives (DQOs) are qualitative and quantitative statements of the quality of data needed to support specific decisions or actions. The quality of the data must be compatible with the decision-making requirements. One measure of the success of a monitoring program is the extent to which the DQOs are achieved. Establishing useful and attainable DQOs depends on identifying the data users; data uses; types of data needed: sampling and analysis options, and parameters related to precision, accuracy, representativeness, comparability, and completeness of the data. Each of these elements is specified in the plan.

Statistical Design

Chemical concentrations in surface water, ground water, soils and rocks can be highly variable in space and time due to various interacting factors, e.g., rainfall, infiltration, runoff, watershed size, soil characteristics, hydrogeology, lithology, recharge and discharge areas, channel size, flow rates, etc. Therefore, the underlying premise of the plan is that background hydrogeochemistry is considered a statistical distribution of concentration levels, rather than a single concentration (Doctor, Gilbert, and Kinnison, 1986).

Statistical Design Criteria

The following statistical design criteria have been developed from the program goals and monitoring and data quality objectives.

0 The data required by the statistical test(s) can be acquired using established methods of sampling and chemical analysis.

0 The test(s) should be relatively easy to perform and interpret.

0 The test(s) should be applicable to a number of indicator parameters representing classes of chemicals.

0 The test(s) should be sufficiently powerful to detect both abrupt shifts and gradual long term trends in the data.

0 The test(s) should be robust or reasonably robust, so that small or moderate departures from the statistical assumptions inherent in the data (e.g., normality, homogeneity of variance, independence) should not significantly affect test performance.

0 The test(s) should be capable of treating non-detected values.

0 The test(s) should be sufficiently reliable to be used in decision-making.

The plan presents procedures for using graphical techniques, tolerance intervals, a test

for trends, and control charts to achieve monitoring objectives, i.e., to determine hydrogeochemical conditions and variability, and to detect hydrogeochemical changes and impacts from waste sites at Rocky Flats. A summary of information expectations including the statistical approach for one of the program goals, an assessment of ground water quality impacts, is presented in Table 1.

Interstation Comparisons

Downgradient and background stations will be compared each time monitoring is performed. Each downgradient concentration will be compared to the range (tolerance interval) of concentrations in background stations. A tolerance interval defines, with a specified probability, a range of values that contains a discrete percentage of the population (U. S. Environmental Protection Agency, 1988). Downgradient stations whose concentrations fall outside the tolerance interval may indicate a release has occurred.

In order to obtain reliable results, both a high level of confidence (95%) and a high percentage of the population within the interval (95%) have been chosen as statistical parameters. A 95% confidence level is considered to provide a reasonable compromise between the probability of Type I and Type II errors (Till, 1974). The number of sampling stations in the background area determines the width of the tolerance interval, i.e., the more background area determines the width of the tolerance interval, i.e., the more background stations, the narrower the interval and the more likely it will be that contamination in downgradient locations will be detected. Nine background stations will define a 95 percent tolerance interval (95% of population within the one-sided interval) with a tolerance factor of three at the 95% confidence level, i.e., the upper limit of the tolerance interval is the mean plus three standard deviations of the sample population. At the end of a year of quarterly groundwater sampling, the power of the test to detect change at downgradient wells will be evaluated. If the power is considered too low, additional wells or more frequent sampling may be necessary.

Tolerance intervals will be used to detect differences between upgradient and downgradient conditions for each sampling event. Control charts and trend tests will be used to detect gradual changes over longer time periods at each station.

Intrastation Comparisons

Comparison of a station's current and past behavior (intrastation comparison) will be used to detect changes over time. The plan proposes the use of time series graphs, trend analysis and statistical control charts for intrastation comparisons. A control chart is a graphical procedure for determining whether the current concentration is above or below control limits established for the station (Doctor, Gilbert and Kinnison, 1986). The control limits are based on historical variability at the station and define typical concentrations in the absence of a trend. Concentrations that lie outside the control limits are considered indicative of a significant change. The control chart itself can often indicate a trend as well as the presence of seasonal data. Control charts will be used to monitor the inherent statistical Yariation in the data, to indicate anomalous results, and to identify possible outliers, data entry errors, or quality control problems. Control charts will be used only if the data are normally or lognormally distributed and serial correlation is absent or moderate.

To detect gradual changes, a sequence of observations rather than individual observations will be examined for trend. The Mann-Kendall nonparametric test is proposed in the plan but the applicability of other trend tests, e.g., Seasonal Kendall test, will be reviewed. A final choice will be made after sufficient data are collected to perform a test. Trend analysis will require at least two years of quarterly data, and will be conducted every year thereafter for key constituents and for each station using the aggregate of all data collected at that time. A key assumption of all trend tests is that the observations are independent. In the absence of a trend, a control chart will be constructed for key constituents at each station. The control chart will establish a range of concentrations

TABLE 1

QUANTIFICATION OF INFORMATION EXPECTATIONS:
GROUND WATER QUALITY IMPACT ASSESSMENT

ıagement Goal:	Determine impacts of facility operations on ground water quality.
ıitoring Objective:	Determine average conditions at background and downgradient wells.
.er Quality Variables:	Concentrations of metals and radionuclides in ground water.
.tistical Methodology:	Compute 95% tolerance intervals (95% of population contained within tolerance interval at 95% level of confidence) for metals and radionuclides at background wells.
.tistical Hypotheses:	Concentrations at downgradient wells are within tolerance intervals at background wells (H_0: DG equal to or less than BG upper limit, H_1: DG greater than BG upper limit).
ıitoring System Product:	Conclusions regarding statistical difference between background and downgradient concentrations.
ıorting Conclusions:	Management goal is met when no statistical difference in concentrations is found (no impact) or when the difference is quantified (impact determined).

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for a constituent at a station so that the latest data can be compared to the range to test if the new datum is within the range (in-control) or outside the range (out-of-control). Control charts will be updated every year provided adjusted quarterly data are not found to be out-of-control during the year.

Data Interpretation

To detect releases from sites, station-specific data will be compared to the range of background concentrations (tolerance intervals), and in the case of surface water and ground water, also compared to the concentrations at the station or well over time.

Soil sampling data will be compared to the background tolerance intervals for that soil type for each monitoring constituent. A soil constituent concentration at a site that is greater than the upper limit of the one-sided 95% tolerance interval at the 95% confidence level will be considered to likely represent contamination.

Determination that a constituent concentration in ground water or surface water represents contamination will be based on 1) comparison of new data to the background tolerance interval, 2) trend testing and/or 3) use of control charts. The utility of trend testing and control charts for downgradient ground-water monitoring data evaluation may be limited because of the possibility that a release has already occurred. The release may not have resulted in a trend and therefore new data will be in-control. At stations where a comparison to background tolerance intervals does not show significant differences, control charts will be utilized. Control limits established for downgradient stations will also be compared to control limits representing the range of background concentrations for key water quality parameters in order to assist in data interpretation.

The minimum data requirement for the statistical tests is one quarter of background data to be used to calculate the tolerance intervals. However, the minimum hydrologic

requirement is two quarters, i.e., a wet or high flow season (spring or early summer) and a dry or low flow season (winter, late summer, or fall) in order to evaluate, at least on a preliminary basis, possible seasonal differences in water chemistry. The assumptions and requirements of the proposed statistical tests will be evaluated against the characteristics of the data. Statistical characterization will include time series plots, calculation of summary statistics (mean, median, variance, coefficient of variation), and testing for normality, homogeneity of variance and independence. Either Dixon's or Rosner's tests for outliers will be used depending on the number of data points available at the time of testing. In general, if an error cannot be identified, the datum will not be excluded from subsequent statistical analysis because the datum may actually reflect greater spatial or temporal variability than expected (background station), or a release from a site (downgradient station). When outliers that are not attributable to errors are contained in the data set, estimators and statistical tests will be computed with and without the outliers to see if the results of the two calculations are markedly different. If the results differ substantially because of outliers in the data, then both results will be reported. If no reasonable explanation for an outlier can be found, and later data are within the normal range for the parameter, the outlier may be excluded but will be noted in the database and in the report(s). When possible or deemed necessary, the sample will be re-analyzed or another sample taken for comparison.

The data obtained from implementation of this plan, including the results of statistical tests, will be interpreted within the context of the overall hydrogeochemical setting. For instance, a particular chemical concentration could be due to a natural but localized event such as storm recharge that results in a statistically significant but erroneous conclusion, i.e., a false positive. Hydrologic and geochemical data will be compared with regional and local precipitation, stream flow, ground-water levels, and water quality records to put the data collected in this investigation and subsequent monitoring in perspective. For example, rainfall and water levels will be

compared to the data record to determine whether they are higher, lower, or average compared to "normal" conditions.

Network Design

Representative background data for surficial materials, bedrock, ground water, surface water, and stream sediments at Rocky Flats Plant will be collected. Sufficient hydrogeologic information has been collected at Rocky Flats to define background regions and subregions. Subregions include areas with different soils, geology and hydrologic characteristics. Different chemistry may be present in subregions. At least one sampling station will be placed in each background subregion. Where multiple sampling stations are placed within a subregion, they have been located to geographically represent the entire subregion. Because depth is expected to influence concentrations in both soils and ground water, soil samples will be taken at different depths, and wells will be completed in surficial and bedrockmaterials. Soils will be sampled once, surface water will be sampled monthly and ground water will be sampled quarterly. The frequency of sampling will be evaluated after collection of a year's worth of data. The data will be evaluated for the occurrence and variability of compounds of interest in time and space. Further discussion of network design, e.g., station locations, frequency of sampling, analytes, or a description of standard operating plans and procedures is outside the scope of this paper.

Reports

Results of the background characterization will be presented in two reports: a background soils characterization report and a background water quality characterization report. Separate reports will be prepared because the data from the one-time soil sampling project will be available much sooner than the two quarters of water quality data to be evaluated for the initial background characterization. The reports will provide the following information: 1) a detailed account of the field investigations including any changes to the plan that may have been necessary due to unexpected field conditions; the geologic/hydrogeologic

characteristics of the background areas with supporting borehole logs, well completions, geologic cross sections and hydraulic test data; 2) the chemical data and a data validation summary including identification and interpretation of any outliers; and 3) an evaluation of chemical data including the computation of background tolerance intervals for soils, ground water, and surface water groups. Reporting of impacts to soil and water quality from Plant operations will be presented in remedial investigation reports for CERCLA sites, closure plans and ground water monitoring reports for RCRA-regulated units, and annual environmental monitoring reports.

SUMMARY

This paper has provided specific guidance on concepts and procedures to assist monitoring system designers in incorporating the following elements into the design process:

1) Identifying and quantifying management goals and information objectives;

2) Establishing statistical design criteria and developing statisticalsampling and data analysis plans;

3) Determining which variables to measure, where to sample, and how frequently to sample considering tradeoffs among goals, information content, operational considerations and budget;

4) Developing sampling, laboratory analysis, quality assurance, data analysis, and data management plans and procedures; and,

5) Developing information utilization and reporting procedures.

Application of the procedures ha been illustrated with a summary of a monitoring plan designed to characterize soil and water quality at an industrial facility.

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Case Study - The TIME Project

THE TIME PROJECT: AN OVERVIEW

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Introduction

This paper is the first in a series of five to discuss the design of the U.S. Environmental Protection Agency's (EPA's) monitoring project to assess the effects of changes in acidic deposition on surface waters of the United States. This project is referred to as TIME (Temporally Integrated Monitoring of Ecosystems).

The TIME project has been in the conceptual and design stage for approximately two years. Delays in implementation have allowed careful attention to many aspects of network design not usually covered prior to field implementation. The network was originally intended as a stand-alone monitoring program, but it has now been incorporated as part of the larger Environmental Monitoring and Assessment Program (EMAP) being planned by EPA.

In this paper, we first discuss the stated goals of the TIME project. We then describe the previous EPA projects relating to aquatic effects of acidic deposition upon which the TIME design is based. In the third section we describe the conceptual model for the sampling design of the project. The last section describes the purpose and contents of the project Data Analysis Plan, which is under development. The four papers that follow describe selected components of the project design in greater detail, including approaches to site selection, types of data to be collected, and identification of appropriate statistical techniques for data analysis.

TIME: Background and Project Goals

Oxidation products of atmospheric emissions of sulfur and nitrogen oxides constitute the main components of acid rain. Anthropogenic emissions of one of these components, sulfur dioxide, have been declining since the early 1970's in the northeastern United States (Husar, 1986). However, little evidence is available to suggest that the rate of lake and stream acidification in these areas has changed (Driscoll et al., 1989; Schindler, 1988). Indeed, although sulfur emissions have declined, nitrogen oxide emissions and deposition have increased, and the net result has been little change in total rainfall acidity (Hedin et al., 1987).

Recent proposals for reducing acidic deposition have targeted sulfur dioxide emissions and call for reductions of 5 million tons by 1995 and for an additional 5 million tons (plus 2 million tons of nitrogen oxide

emissions) by the year 2000. These reductions will leave sulfur dioxide emissions at approximately 60 percent of current emissions. To achieve this level of control, the proposed reductions require funding commitments of approximately $700 million per year by 1995 and $3.8 billion per year by 2000. Given the magnitude of this investment, it is appropriate that a well-designed long-term monitoring program be in place to assess the effectiveness of this decrease in emissions on aquatic resources currently affected and at risk of further degradation.

The TIME project is intended to:

- provide early-warning signals of surface water acidification (or recovery) in regions of interest,

- provide an ongoing assessment of regional patterns or trends in surface water acidification (or recovery),

- assess the relationships between observed patterns and trends in surface water quality and observed patterns and trends in atmospheric deposition, and

- assess the extent to which observed patterns and trends in surface water chemistry correspond with model forecasts of surface water chemistry.

TIME has been designed to collect long-term data, both chemical and biological, on acid-sensitive lakes and streams in areas of the United States considered potentially susceptible to the effects of acidic deposition (Thornton et al., 1987; Payne and Ford, 1988). The project is designed to use information on wet deposition available through existing monitoring networks that may be augmented to meet project goals. As of June 1989, the project was scheduled for implementation in the spring of 1991.

Related EPA Studies on the Aquatic Effects of Acidic Deposition

The TIME project focuses on regions of the United States where there are lakes and streams with low levels of acid neutralizing capacity (ANC). These sensitive regions have

been identified and studied in two types of major projects now underway or recently completed by EPA's Aquatic Effects Research Program (AERP). The first type includes large-scale surveys designed to identify the status and extent of surface water acidification in the United States. The second focuses on more detailed characterization and process-oriented research on selected systems, in an effort to provide an understanding of the underlying mechanisms responsible for the regionally observed patterns and effects. We briefly describe here those surveys and projects most closely related to the TIME project design.

The regional studies are collectively known as the National Surface Water Survey (NSWS). The NSWS consists of two main components, the National Lake Survey (NLS) and the National Stream Survey (NSS). The NLS in turn consists of two major regional surveys, the Eastern Lake Survey (ELS; Linthurst et al., 1986 and Landers et al., 1988) and the Western Lake Survey (WLS; Landers et al., 1987 and Eilers et al., 1988). The purpose of these regional synoptic surveys, all of which have now been completed, was to provide a snapshot characterization of the populations of interest. The regions surveyed in each of these projects are shown in Figure 1.

The Eastern Lake Survey was conducted in two phases. In Phase I, 1798 lakes were sampled once during the fall turnover period in 1984 in the Northeast, Upper Midwest, and Southeast. Phase II of the survey was conducted in 1986; 145 of the lakes sampled in the Northeast in Phase I were sampled once in each of the spring, summer, and fall seasons. During the Western Lake Survey, 719 lakes in the mountainous areas of the western United States were sampled during fall turnover in 1985. The WLS was recently augmented by the Kenai Lakes Investigation Project (KLIP), during which 59 lakes on the Kenai Peninsula of Alaska were sampled during August 1988 (Ford et al., 1988; Landers et al., 1989).

The NSS also was conducted in two phases. In the first phase, a pilot survey, 54 stream reaches were sampled in the spring and

WEST

NORTHEAST

UPPER MIDWEST

MID-APPALACHIANS

MID-ATLANTIC

INTERIOR SOUTHEAST

FLORIDA

KENAI LAKE INVESTIGATION PROJECT

NATIONAL LAKE SURVEY (NLS)

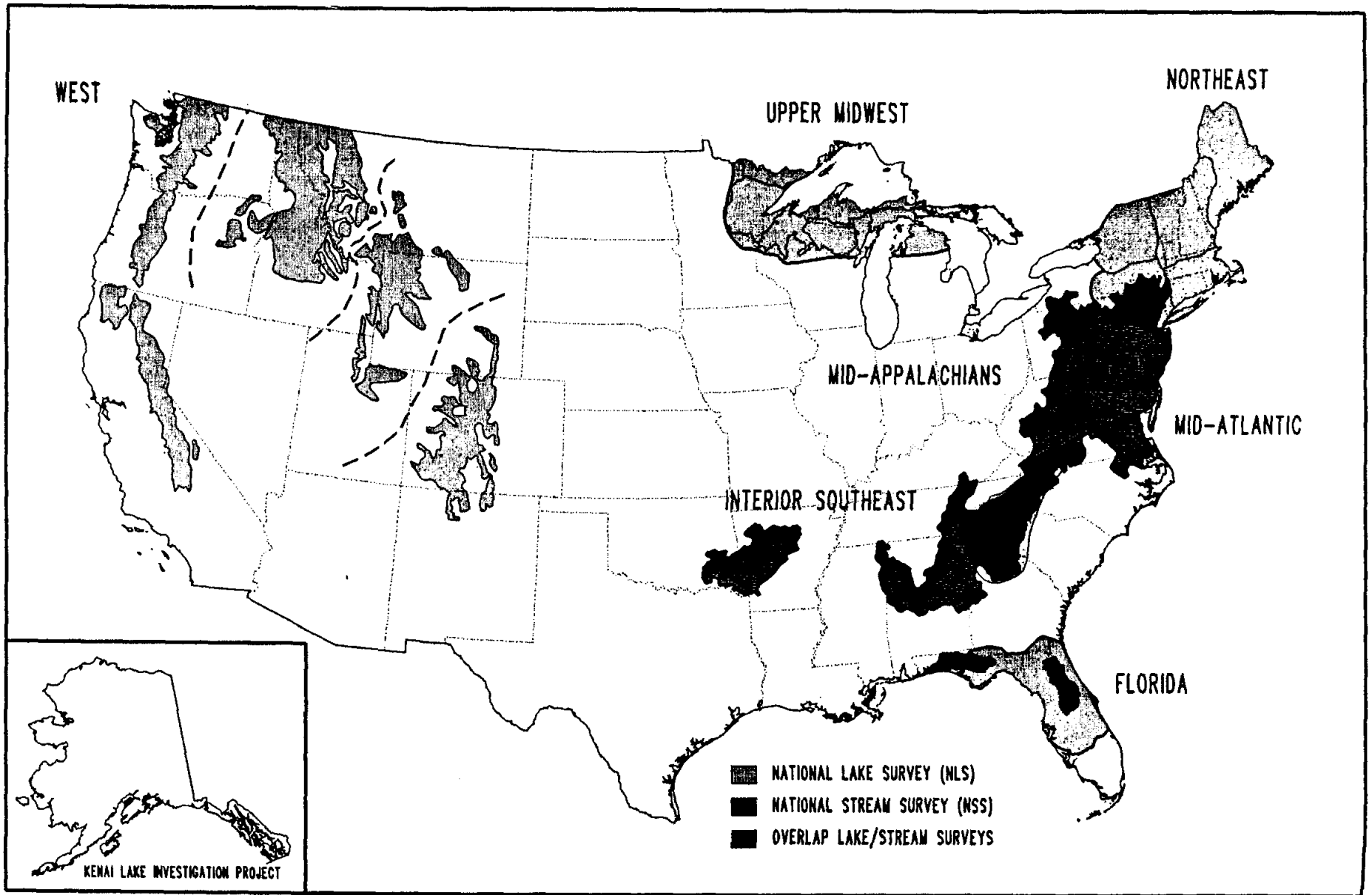NATIONAL STREAM SURVEY (NSS)

OVERLAP LAKE/STREAM SURVEYS

FIGURE 1. Regions of interest in the National Surface Waters Survey.

summer of 1985 in the Southern Blue Ridge to assess the logistic and scientific feasibility of a full-scale survey (Messer et al., 1986; 1988). The full survey was then conducted in the Mid-Atlantic and Southeast in the spring of 1986, when upstream and downstream reach ends were sampled at 445 stream reaches (Kaufmann et al., 1988).

The NSWS surveys were designed to be statistically representative subsets of the population of resources at risk. For the NLS, the lake population was divided into strata defined on the basis of region, subregion, and preliminary versions of mapped alkalinity class (Omernik and Powers, 1983; Omernik and Kinney, 1985; Omernik and Griffith, 1986a, 1986b), and a systematic sample of lakes was drawn within each stratum. The NSS also was stratified by region and subregion, but because listing the extensive number of streams was not feasible, a two-stage sampling scheme based on a point frame within strata was employed. Thus, in both the NLS and the NSS, systems were selected for sampling within subregions with known, but unequal, probabilities (Blick et al., 1987). This design allowed for determination of the percentage (by number and area), location, and chemical characteristics of surface water populations in potentially sensitive regions and subregions. The probability sampling approach also provides both context and rationale for selecting lakes and streams for longer term monitoring for acidic deposition effects.

One of the objectives of the NSWS was to determine the proportion of lakes or streams having a certain chemical value less than or equal to a specified value. Such a proportion is easily estimated as the ratio of the estimated number of lakes (or streams) that meets that criterion divided by the estimated number of lakes (or streams) in the population of interest. This ratio can be calculated for the whole range of criteria encompassed by the data, and can be plotted as a relative cumulative frequency curve; curves can then be overlain to compare characteristics of regional or subregional populations. Figures 2a and 2b are examples of these curves for ANC in lakes in all NLS regions and in WLS subregions, respectively. Median ANC values can be compared by extending a horizontal line from

0.5 on the ordinate; thus in Figure 2a we see that median ANC is lowest in Florida (about 75 μeq/L) and highest in the Upper Midwest (about 350 μeq/L). The proportion of lakes with ANC less than 200 μeq/L can be compared by extending a vertical line from 200 on the abscissa; in Figure 2b, for example, we see that about 85 percent of the lakes in the California subregion and about 40 percent of the lakes in the Southern Rockies subregion have ANC values below this critical level.

The Direct/Delayed Response Project (DDRP) (Church 1989) was implemented after NSWS sampling and was intended to provide an understanding of the underlying mechanisms responsible for the observed patterns in surface water chemistry. Under DDRP, regional soil surveys were made on statistically representative sets of watersheds consistent with the NSWS, and three models of surface water acidification or recovery (MAGIC, ILWAS, and Enhanced Trickle-Down) were applied in order to predict changes in surface water chemistry likely to occur under various sulfate deposition scenarios (Jenne et al., 1989).

The Long Term Monitoring (LTM) project was initiated in 1982 to follow trends in surface water chemistry of systems with low ANC across national and regional gradients of atmospheric sulfate deposition (Newell et al., 1987; Ford et al., in preparation). This is a cooperative project, in that EPA has supported federal, state, and university researchers in chemical monitoring of 90 lakes and streams. These surface water systems are located across the northeastern and northcentral United States as far west as Colorado (Figure 3), and are typically sampled monthly or seasonally. A more complete description of the current configuration of the LTM project may be found in Ford et al. (in preparation). It is expected that many of the LTM systems will be selected for continued monitoring under the TIME project.

Conceptual model of the TIME Project

The conceptual model for the TIME project, which is sometimes referred to as a "wheel and axle" design, is depicted in Figure 4. The left side of the figure represents the
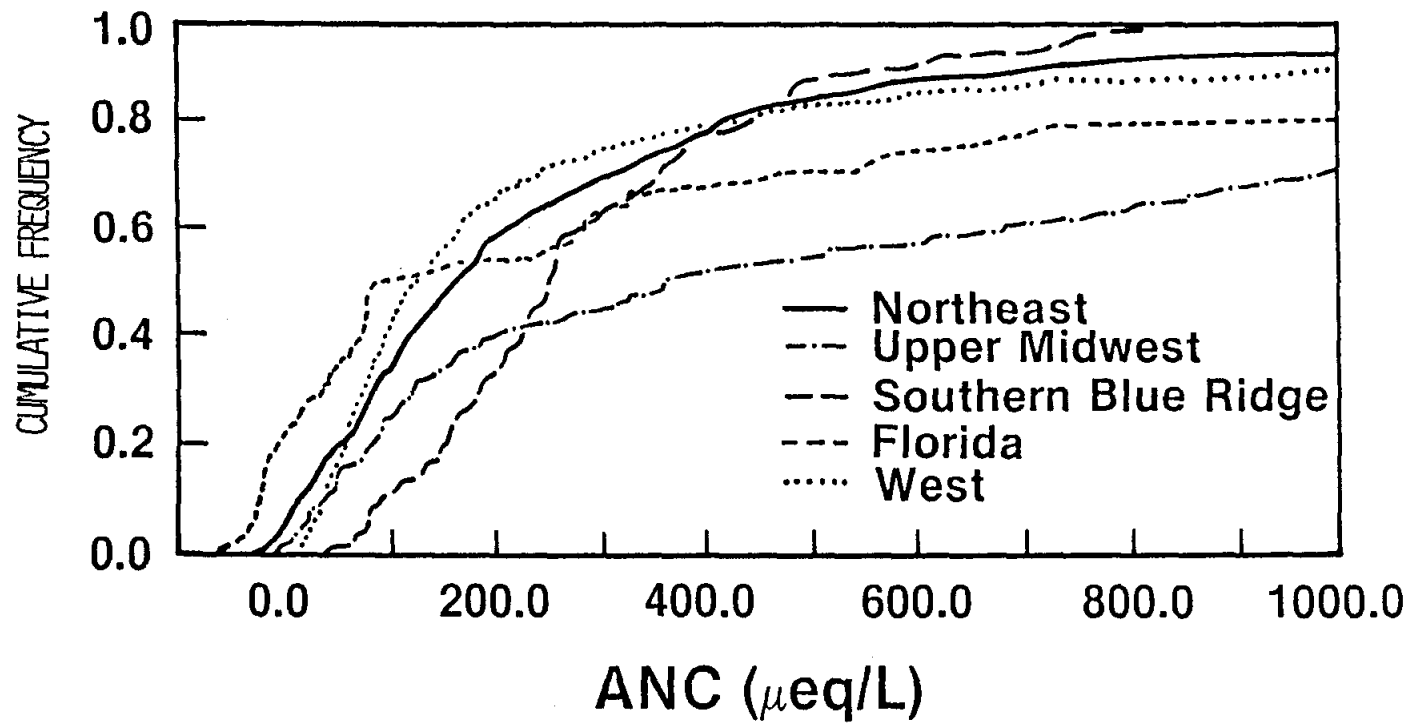
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FIGURE 2a. Cumulative frequency distributions for acid neutralizing capacity in National Surface Water Survey regions.
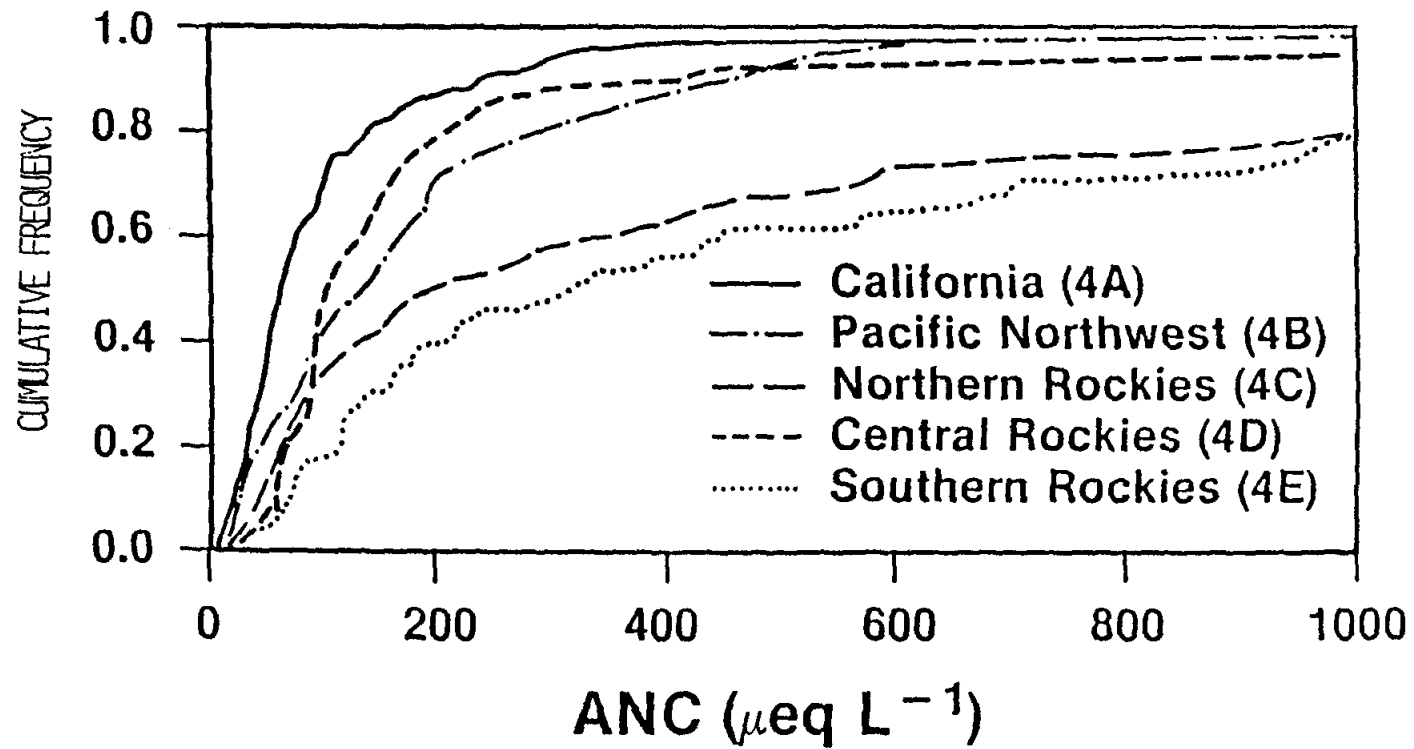
FIGURE 2b. Cumulative frequency distributions for acid neutralizing capacity in lakes in subregions of the Western Lake Survey. Source: Landers et al., 1987.
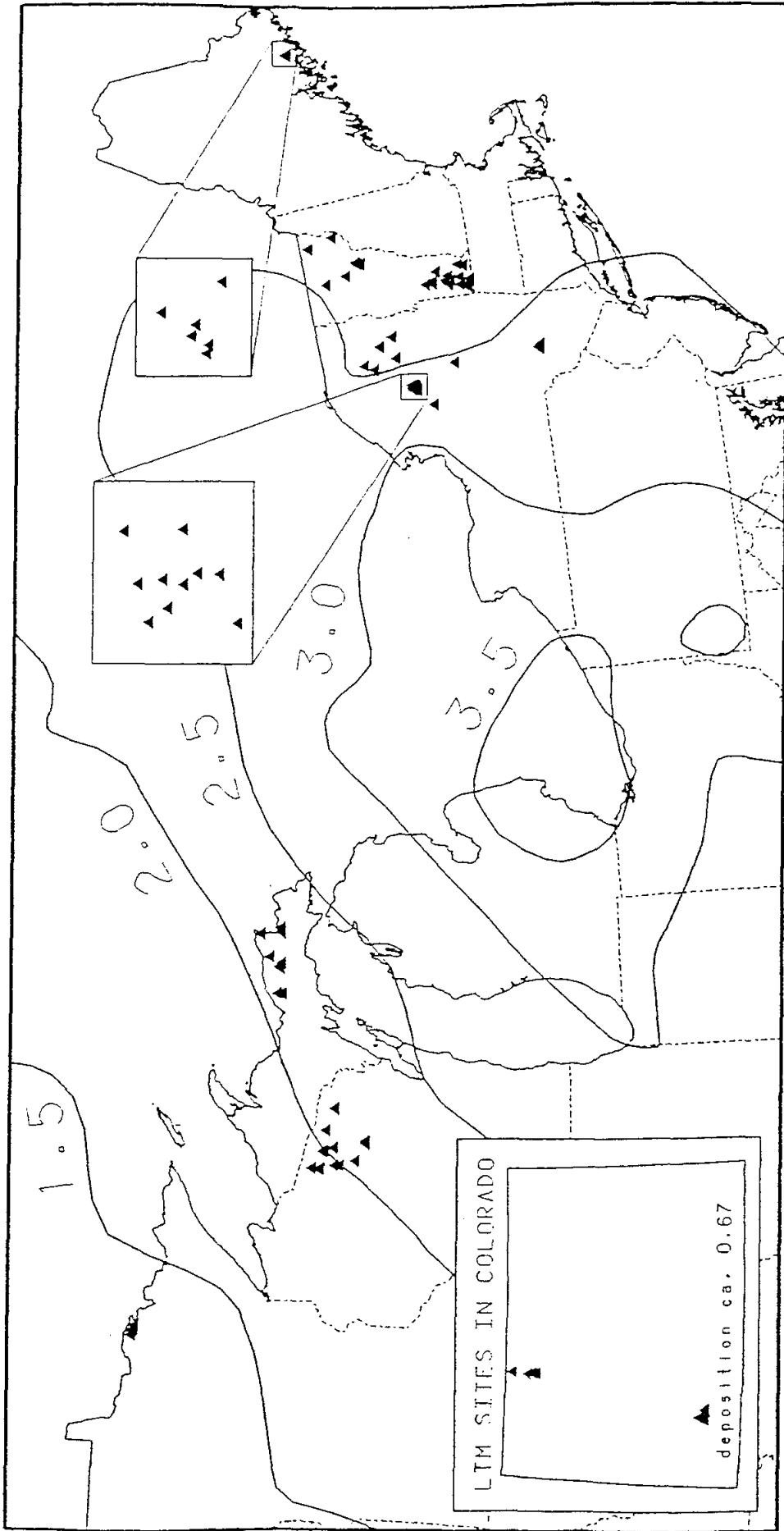
Fig. 3 LONG TERM MONITORING SITES WITH WET SO$_4$ DEPOSITION CONTOURS
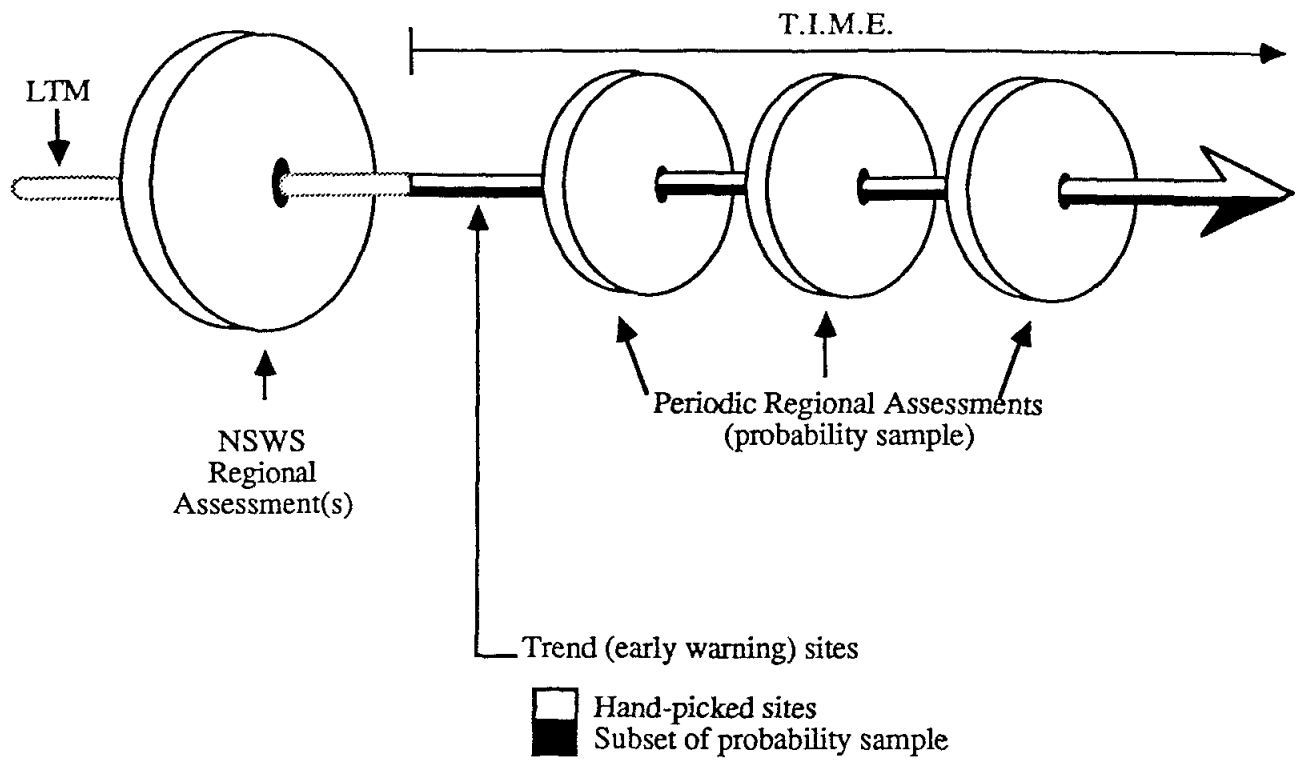(g/m^2 per year, 1980-1984)

FIGURE 4. Temporally Integrated Monitoring of Ecosystems (TIME) project conceptual "wheel and axle" model.

existing NSWS program elements upon which the TIME project will be built; the axle represents the temporally intensive LTM project and the wheel represents the statistically representative regional surveys. The right side of the figure represents proposed sampling under the TIME project. The axle, or early-warning, systems will be chosen to represent ongoing monitoring of highly sensitive resources that are expected to respond rapidly to changes in acidic deposition (Young and Ford, 1989). The wheels are designed to provide periodic assessments of status and trends for particular geographic regions of interest. Combining temporally intensive and regionally extensive elements in the TIME design balances the need for regional assessments with the need for ongoing monitoring of rapid response systems for networks addressing specific pollutant impacts such as acidic deposition.

As shown in the figure, the two types of early-warning systems include hand picked sites with pre-existing data (these may be selected from, but are not limited to, LTM systems), and probability sites chosen from appropriate subsets of the NSWS. For axle systems that are not elements of the NSWS (referred to as "found" sites), the relationship between these sites and sites in the NSWS population will be described using a model-based approach (Overton, 1989). Each early-warning system will represent a subset of the population; significant chemical and/or biological changes in an early-warning system will prompt further study of the corresponding subset in the population. The purpose of sampling these systems more frequently is to provide an ongoing assessment of significant changes in surface water quality of rapid response sites related to changes in acidic deposition as well as to assess patterns and trends in seasonal and annual variability necessary to interpret trends.

The periodic regional assessments can easily be developed as resurveys of subsets of NSWS sites. One possibility for the eastern U.S., for example, would be to focus sampling on the DDRP sites in the Northwest, Mid-Atlantic, and Southern Blue Ridge Province. Regional assessments can follow the original NSWS protocol, with a single sampling effort

during an "index" period of relatively stable water chemistry (e.g., fall turnover for lakes, spring baseflow for streams), with sampling intervals between regional surveys determined by results from the early-warning systems, regional needs, and budgetary constraints.

The TIME Data Analysis Plan

The Data Analysis Plan is being prepared as part of the planning and design of the TIME project. The purpose of this document is to describe the statistical analyses that will be performed to address the major research questions of interest. By initiating these activities well in advance of actual field implementation, the needs of prospective methods of data analysis can be incorporated into the actual design of the monitoring network. The kinds of decisions that could be influenced by these activities include the number and geographic distribution of surface water and deposition sites, the frequency and amount of replication of sampling efforts, and the number and types of quality control samples.

The technical chapters and the primary issues to be addressed in each are as follows:

- Trends in individual surface water systems. How do we assess whether or not there are meaningful statistically significant changes over time in a specific variable for an individual system, given the available data? In a vector of variables?

- Trends in regional populations. How do we characterize given variables for populations of interest in a region or subregion? How do we compare the distribution of a variable between two time periods? How can univariate and multivariate trends in regional populations of surface water systems be estimated, and how do we assess whether or not the observed trends are statistically significant and ecologically meaningful?

- Trends in biological parameters. What biological response variables should be used to assess important biological

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changes over time? Which response variables are best for early-warning signals, which are best for regional assessment of change from one time period to another, and which are best for detecting biological trends over time? How do we assess, at a given point in time, whether or not these biological response variables have gone below or exceeded a critical level? What statistical techniques are appropriate for the assessment of changes over time in the biological response variables of interest?

- Integration of non-NSWS surface water systems into NSWS populations. How do we determine the subsets in the probability sample that are represented by the individual (axle) surface water systems? To what extent can we extrapolate observed changes in individual surface water systems to changes in subpopulations within a region? To what extent can we use observed variability in trends in individual or groups of axle systems to estimate variability in the subpopulation trends?

- Trends in deposition. Can deposition to axle systems be adequately represented by data from existing deposition monitoring sites? How representative are the regional deposition networks of the TIME regional populations? How do we estimate and test the statistical and practical significance of trends in deposition at individual stations? How do we estimate and test the statistical and practical significance of regional deposition trends?

- Relationship between trends in deposition and trends in surface water chemistry. How do we assess whether or not there are statistically and practically significant relationships between changes in deposition and changes in surface water chemistry in an individual surface water system?

Between changes in deposition and changes in surface water chemistry in a region?

The technical chapters in the Data Analysis Plan will describe and provide sample applications of the approaches recommended for data analysis by cooperating researchers, descriptions of other approaches considered, and justifications for the selection of recommended approaches. The assumptions and sensitivity of analytical results to these assumptions also will be described.

The Data Analysis Plan is intended to be read by a wide audience; thus the recommended techniques will be explained at a level understandable by scientists and decision-makers with a knowledge of basic statistics. Appendices to the document will describe the recommended techniques in greater technical detail for these who are interested. In particular, the Appendices are intended to be sufficiently detailed so that TIME data analysts, database managers, and programmers can use them as guides to implementation of recommended techniques.

The four papers that follow represent contributions to these elements of the TIME Data Analysis Plan, and describe in detail selected components of the TIME project design and data analysis approaches. The first, by Young and Ford, describes a process by which the NSWS data base can be analyzed to optimize site selection for both the early-warning and the regional assessment components of the TIME design. Daly then discusses a conceptual plan for estimating wet deposition to TIME regions and early warning sites and assessing the adequacy of existing deposition monitoring networks for representing deposition to these regions and sites. The next paper, by Hughes, describes the types and uses of biological data that can be collected for the purpose of assessing the biological effects of surface water acidification or recovery. The last paper, by Loftis and Taylor, describes recommended approaches for detecting univariate trends in individual surface water systems. Extensions of this work to multivariate trend detection is in progress.

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SITE SELECTION PROCEDURES FOR TEMPORALLY INTEGRATED MONITORING OF ECOSYSTEMS (TIME)

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ABSTRACT

A long-term program to monitor aquatic ecosystems requires a long-term commitment of significant resources. To maximize the effectivess of such a program, monitoring sites must be carefully selected, addressing a complex array of relevant concerns in the process. Monitoring sites for the TIME Project (Temporally Integrated Monitoring of Ecosystems), scheduled to begin in 1991, will be selected for chemical and biological sampling in order to meet several distinct objectives, including (1) establishing an "early warning" network to detect changes in aquatic resource acidification or recovery, (2) providing periodic regional assessments of surface water acidification status, (3) providing data for validation of watershed models, and (4) relating surface water responses to atmospheric deposition. This paper focuses on a method for selecting sites to meet the first objective for lakes and does so using data from the National Surface Water Survey (NSWS). The approach involves a cluster analysis to stratify the NSWS sample and ordination to identify lakes that are likely to respond to changes in acid inputs.

BACKGROUND AND ISSUES

The most extensive information on the current status of surface water acidification in the United States derives from recently completed efforts by the U.S. Environmental Protection Agency (EPA). Under the aegis of the National Acid Precipitation Assessment Program (NAPAP), EPA conducted the National Surface Water Survey (NSWS) during the mid-1980's. This program included the National Lake Survey (NLS) and the National Stream Survey (NSS). The results of these efforts have been reported in detail (Linthurst et al. 1986, Landers et al. 1987, Kaufmann et al. 1988). It is clear from these surveys that poorly buffered surface waters occur widely and that systems located in regions of high acidic deposition evidence the greatest degree of acidification (Landers 1988, Eilers 1988).

Among existing water quality monitoring programs, few have combined regional and temporal design elements in a manner that is adequate to determine the effects of declining emissions on aquatic systems, and none have been designed specifically to meet that objective. The EPA's Long-Term Monitoring Project (LTMP), a major effort that pertains to lake ecosystems likely to respond to deposition changes, incorporates some spatial and temporal analysis (Newell et al. 1987, Ford et al. in prep.). LTMP involves seasonal to monthly sampling and analysis for acidic deposition effects on nearly 100 lakes in the northeastern, midwestern, and western

United States. LTMP lakes were not selected randomly, however, so they do not represent explicit regional lake populations or subsets, in contrast with the NSWS lakes (Blick et al. 1988; Pollack and Ford, this issue). As a consequence, changes in water quality status and trends observed in LTMP lakes cannot be interpreted without bias as representing the average response of the regions in which they are located.

EPA's TIME Project (Temporally Integrated Monitoring of Ecosystems) seeks to bridge the design gap that exists between the NSWS and the LTMP projects and, in so doing, provide the information needed to assess the effectiveness of emissions controls on acid-sensitive aquatic systems. By building on experience gained during the NSWS and LTMP efforts, the TIME Project will integrate spatial with temporal monitoring. In the introductory paper to this symposium session on the TIME Project, Pollack and Ford (this proceedings) describe the goals of the TIME Project. This paper provides an overview of the process that will be used to guide selection of monitoring sites as the first step in achievement of these goals. While the TIME Project includes monitoring of streams as well as lakes, the focus of this paper will be on the selection of lake systems.

APPROACH

The main goals of the TIME Project have been given by Thornton et al. (1987) and also by Pollack and Ford (previous paper). The goals also have been stated as specific project objectives (Thornton et al. 1987). These objectives are restated here to give a point of focus for discussing site selection procedures. The objectives of TIME are to:

1. Provide early detection of changes in surface water acidification in regions of interest.

2. Provide periodic assessments of regional patterns and trends in surface water acidification status.

3. Determine the degree to which chemical and biological patterns and trends correlate between surface waters observations and watershed model forecasts.

4. Determine the degree to which chemical and biological patterns and trends correlate between surface waters and atmospheric deposition.

Objective 1

The first project objective will require monitored sites that provide early detection of changes in acid-base chemistry. Such systems must be highly responsive to acidic loadings to minimize the time required to detect trends and changes in acid-base status.

A significant obstacle to selecting monitoring sites that are especially sensitive to acid and base loading is the need to define aquatic system characteristics that will permit early detection of change by satisfactory monitoring procedures. This difficulty is discussed more fully in a later section, but an example is useful here. A measurement of water column pH gives a direct indication of free acidity in an aquatic system, so a superficial view might conclude that pH would serve well as an indicator of sensitive systems for TIME Project monitoring. Water column pH, however, may be relatively stable at high or low values depending on the buffering provided by other aqueous chemical components. Consequently, water column pH provides an ambiguous criterion for ranking lake sensitivity to acid and base inputs. To make the example more specific, pH in very low ANC (acid neutralizing capacity) systems may be buffered by aluminum hydrolysis or humic substance protolysis. The pH in aquatic systems with these attributes would be low but comparatively unresponsive to changes in acid or base inputs. Thus, robustness of the selected parameter for defining sensitivity is important. Furthermore, the parameter should be measureable with relatively high simplicity, precision, and accuracy to measure to increase the likelihood of its presence in datasets of interest.

The lake and stream populations that formed the basis for NSWS site selection will

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comprise the main populations of interest to the TIME Project. The known statistical attributes of these populations make the NSWS sites particularly desirable for some purposes (see Objective 2). Nonetheless, non-NSWS monitoring sites ("found" sites, Overton 1989), also will be considered for selection if the data collected to date are especially relevant and of high quality.

It may be neither possible nor necessarily desirable to select monitoring sites solely and randomly from NSWS lake groups (strata) formed on the basis of early detection criteria. Such a constraint on site selection would be necessary to yield unbiased estimates of change in lakes within large geographic regions (Objective 2). However, randomly selected sites may not be efficient at guaranteeing inclusion of lakes that are most sensitive and, therefore, best able to provide early warning of change. Rather, a purposive ("hand-picked") sample may be most useful for early detection of deposition-related changes in water quality, depending on (1) the number of lakes from which sites may be selected, (2) the number of lakes upon which projections are to be cast, and (3) how much prior information is available on the lakes.

Objective 2

In contrast with the possible use of nonrandomly selected sites for meeting the first objective, determining temporal changes in surface water acidification for large geographical regions will require randomly selected sites from the region of interest. Statistical population frames (enumerated lists of all possible sampled sites) for both streams and lakes in regions of high suspected effect from or sensitivity to acidic deposition were developed for the NSWS. These frames will be used for site selection by the TIME Project.

It is expected that the selection process for lakes will follow an approach similar to that used to estimate temporal changes in acidification in the northeastern United States during the NSWS (Phase II of NLS; Thornton et al. 1986, Overton 1987). In order to implement this approach, known as double sampling (Cochran 1977, Overton 1987), the

sample of lakes selected for regional lake status characterization (Phase I of NLS) will be restratified based on sensitivity and response parameters developed to select early detection sites for Objective 1. Subsequent to restratification, a suitably-sized, random sample of sites will be drawn and reweighted for parameter estimation as required by the Phase I and restratified sample characteristics (Overton 1987).

Objective 3

The third objective requires monitoring of sites that have been included in EPA's forecast modeling efforts. Of particular interest are the lakes (a random subsample of the NLS Phase II lakes) that formed the target systems for EPA's essentially completed Direct-Delayed Response Project (DDRP, Church et al. 1989). DDRP is an extensive catchment-receiving water characterization and modeling project focused on the northeastern and southeastern United States Although the DDRP will not achieve formal completion until 1990, much of the modeling activity has concluded (Church et al. 1989). Accordingly, modeling forecasts of water quality sensitivity and response to a range of future acidic deposition scenarios, ranging from a few years to several decades, are available for all included systems. Consequently, TIME monitoring sites selected from DDRP lakes can include systems for which forecasts indicate early response, as required to meet Objective 1. Selection specifically on the basis of forecast characteristics, however, eliminates the element of randomization from the selection and precludes the use of such lakes for regional acidification estimates.

Objective 4

Assessment of relationships between trends in surface water response and deposition chemistry ideally requires surface water monitoring sites in proximity to deposition monitoring sites. Purposive selection of early warning sites, a protocol likely to be used for a fraction of TIME monitoring sites, can also ensure some degree of achievement of the proximity requirement. But, as discussed by Daly (this issue), a major issue facing the TIME Project is the adequacy of existing

monitoring networks (e.g., the National Atmospheric Deposition Program/National Trends Network) for providing sufficiently accurate deposition data for meeting Objective 4. If existing networks should prove to be inadequate, the TIME Project will recommend installation of additional deposition monitoring sites and provide recommendations on site locations.

In summary, the TIME Project will use water quality monitoring sites that include both randomly and purposively selected systems. Sites chosen randomly from the NSWS sampling frame, after restratification, will enable estimation of regional response to deposition in terms of chemical and biological trends and changes in status through time. On the other hand, early detection of changes in surface water acidification, assessment of model predictions, and determination of relationships between surface water response and deposition chemistry have need of sites selected with prior knowledge of candidate systems chemical and biological characteristics.

SPECIAL CONCERNS IN SITE SELECTION

Inclusion and Exclusion

In addition to factors derived directly from primary project objectives, other factors that indirectly relate to the objectives (Table 1) also affect site selection. Some of these factors will be addressed within the TIME Project by applying formal rules for inclusion and exclusion of candidate monitoring sites. Although these rules are not addressed explicitly here, published descriptions of site selection protocols for the NSWS (Linthurst et al. 1986, Landers et al. 1987, Kaufmann et al. 1988) provide entirely relevant examples of criteria that would apply to selection of TIME monitoring sites.

A special concern on the list given in Table 1 is that of watershed disturbance. The TIME Project specifically addresses questions related to changes in water quality attributable to changes in acidic deposition. As a consequence, uncontrollable, confounding influences on water quality, as would accompany human activities in a watershed, should be avoided or at least minimized to the extent possible.

"Found" Monitoring Sites

In the preceding discussion of project objectives and site selection, several issues were identified that have particular importance to the TIME Project. One is the problem of whether and how to make regional population estimates using data from monitoring sites selected in part by exercising a probability protocol, such as, random sampling from an explicit frame, and in part by a nonprobability selection, such as, picking sites in a region on the basis of length of pre-existing record.

Often the difficulty of monitoring sites selected by a nonprobability procedure is compounded by a lack of recognition that a problem exists in data interpretation. A simple example will illustrate the nature of the situation. Given a monitoring program for a region based on a random sample of 20 lakes, why should ANC data available from a local researcher on a particular lake in the region (not part of the random sample) be excluded from estimates of the regional mean lake ANC? Perhaps it should not. Generally speaking, however, the local researcher's reasons for picking the site will not duplicate those of the regional monitoring program. Thus, the primary obstacle to including the local researcher's information is a lack of knowledge about the "representativeness" of the lake for estimating the regional chemistry. The representativeness of the random sample, on the other hand, is not in doubt if selected according to protocol.

As explored by Overton (1989), statistically rigorous procedures can be developed that permit "found sample" inclusion on the basis of an informed judgement on representativeness. These procedures, however, will require more testing before their general usefulness can be established.

Early Detection and Restratification Criteria

An essential issue for the TIME Project is the identification of aquatic system characteristics that permit early detection of acid-base status changes and that may be monitored satisfactorily. One approach to identification of suitable characteristics, and

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Table 1. Ancillary factors affecting site selection for the TIME project.

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*   Watershed disturbance

     - Road salt from deicing activity

     - Chemical manipulation (e.g., limestone neutralization)

     - Land use (agriculture, habitation, transportation, and others)

*   Length and quality of pre-existing chemical record

*   Intensive or extensive monitoring effort at site

*   Suitability for both chemical and biological monitoring

*   Flexibility for meeting future changes in research focus or level of activity

*   Likelihood that region will experience a significant change in deposition

*   Accessibility for sampling

*   Regional heterogeneity or presence of spatial gradients

*   Special conditions and value of data if site was selected by a nonprobability protocol

     - Lake or watershed area

     - Soil type

     - Hydrologic regime

     - Indirectly related research interest

_____

the one followed here, is to consider information that reflects the sensitivity and past response of candidate systems to acidic deposition. Given the identification of suitable water quality characteristics, relevant data on the candidate sites will allow their classification into sampling strata. Subsequently, sites may be randomly selected from one or more strata for inclusion in the monitoring program, subject to application of the exclusion criteria mentioned previously.

The NSWS database contains a wealth of information related to the acid-base chemistry of lakes and streams that may be used to characterize the sensitivity and response of those systems and their potential usefulness for early detection of change in status. One view of a small subset of the available information is shown in Figure 1, which illustrates the relationship between bicarbonate ion and divalent cation concentrations in drainage lakes in Regions 1 (Northeast) and 4 (West) of the NLS. Regions 2 (Upper Midwest) and 3 (Southeast) were not included on Figure 1 to reduce data density for plotting. These data indicate the existence of a strong linear association (approx. 1:1, equivalent basis) between these quantities in a majority of lakes, particularly in Region 4. Also, a strong divergence from this pattern was evident, mainly in lakes from Region 1. The divergence is consistent with the pattern expected from a catchment-receiving water system wherein strong acid anions, such as sulfate or nitrate, or organic ligands have replaced bicarbonate in the electroneutrality balance.

Based on the assumption that divalent base cations, particularly Ca, and bicarbonate ion generally share geochemical origins (the weathering of carbonate bearing minerals), these data suggest the occurrence of lake response to acid inputs. Clearly, precipitation sources of acids cannot be distinguished from natural sources from these data, but the geographical distribution of the apparent ion replacement (Northeast > West) is consistent with that of precipitation sources of acids (Husar 1986). The lowest concentrations of bicarbonate occurred in lakes that contained comparatively high divalent cation levels. Hence, considering the entire NLS results, the

lakes with the greatest apparent response to acid inputs (least bicarbonate relative to divalent cation levels) formed a separate group from those with the greatest apparent sensitivity to acid inputs (least bicarbonate present in amounts equivalent to divalent cation concentrations). Based on this characterization scheme, it appears that lakes in the northeast include most of the high response systems, while high sensitivity lakes (divalent cations equivalent to bicarbonate ion concentrations, low concentrations) comprise the majority of systems in the west.

Sensitivity and response inferences such as these will be used in the process of selecting TIME monitoring sites. The nearly 1100 member drainage lake subsample from NSWS Regions 1 and 4, depicted in Figure 1, can facilitate a simple demonstration of the workings of a strategy that uses sensitivity and response information. This data subset, of course, neither includes lakes from all United States regions of interest regarding acidic deposition, nor considers hydrologic types other than drainage lakes.

Drainage lakes may be partitioned objectively into a number of subgroups, or clusters by applying a classification algorithm to individual lake characteristics contained in the NSWS database. The lake characteristics selected for clustering may include, but need not be limited to, variables selected to quantify sensitivity and response. Including a variety of limnological variables in the cluster analysis, rather than just those that reflect sensitivity or response to acidic deposition, results in clusters that more broadly define lake subpopulations present in the NSWS sample. Such a multivariate clustering, however, will have less power to discriminate between sensitive and responsive lake classes, compared to clustering, for example, on ANC alone. This develops because the multivariate strategy uses additional variables to define lake categories, and the additional dimensions of variance decrease distinctions among clusters.

After lake clusters are formed, those that rank highly on the sensitivity and response variables may be subsampled, randomly if desired, to provide a selection of monitoring

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Drainage Lakes of the National Lake Survey
Regions 1 (Northeast) and 4 (West)
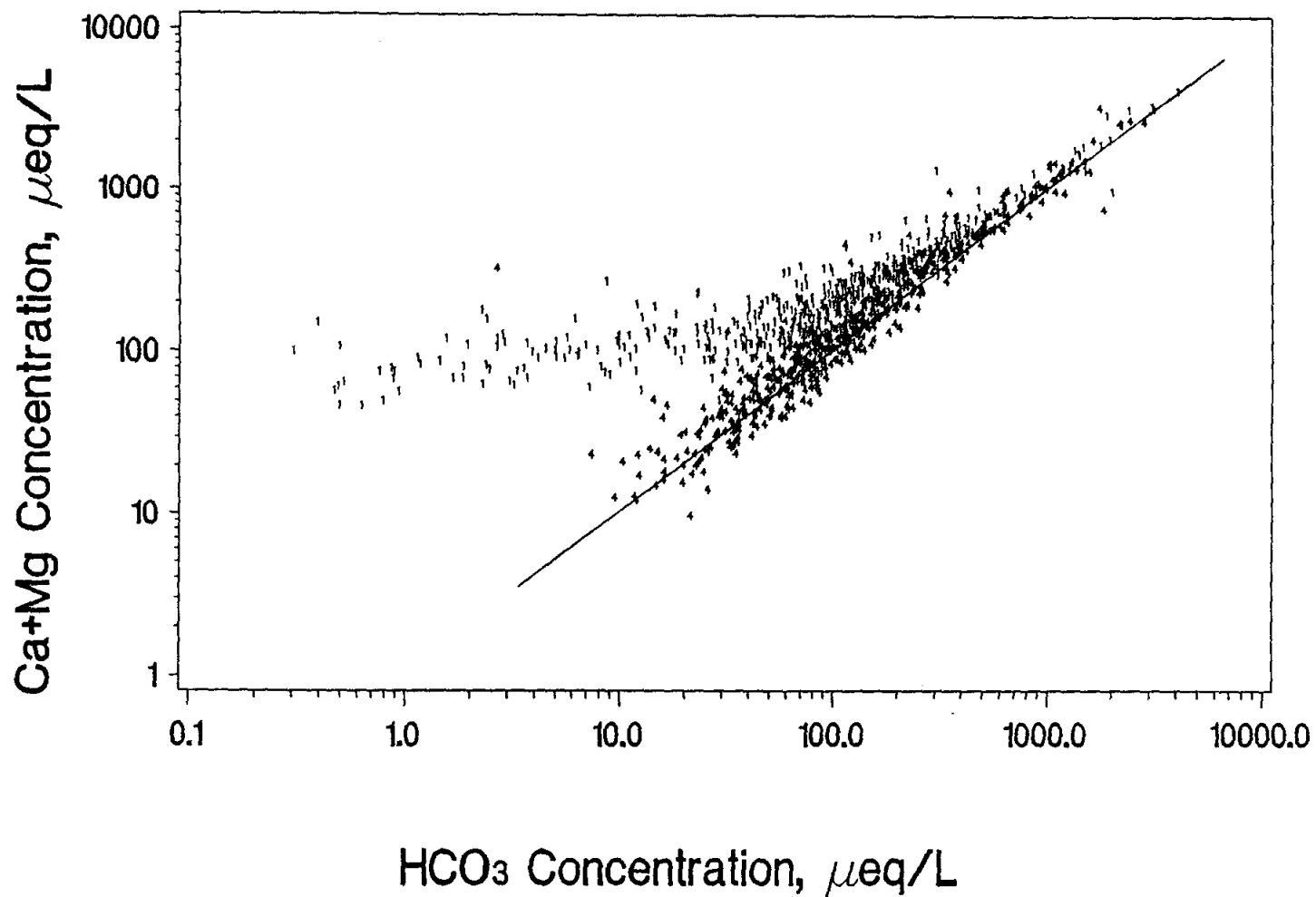
HCO3 Concentration, μeq/L

Figure 1.   Relationship between equivalent concentrations of major divalent base cations and bicarbonate anion in drainage lakes of the northeast and western United States; straight line has 1:1 slope; data from National Surface Water Survey (Linthurst et al. 1986, Landers et al. 1987).

sites that may be considered representative of the sensitive or high response lakes. The number of lakes desired for monitoring may exceed the number available in a single cluster, so selection of more than one cluster may be needed to fill the sample. In this case, the most sensitive or highest response cluster may be censused if desired, or the subsampling process may be extended to multiple clusters to provide broader representation of lake classes in the monitoring program.

The lakes represented in Figure 1 were partitioned into eight subgroups by a nonparametric cluster analysis (Two-Stage, Kth Nearest Neighbor Density Algorithm; SAS Institute, Cary, NC) using log-transformed lake concentration data for total alkalinity, dissolved organic carbon (DOC), and the ions: chloride, hydrogen, and sulfate. The results of the analysis are summarized in Figure 2, wherein circles identify the position of lake clusters. The center of each circle marks the cluster mean for divalent cations and bicarbonate ion, and each circle diameter is proportional to the number of lakes in the cluster (cluster membership). The multiple-member clusters are identified by letter; the largest of these has 266 lakes while the smallest has 18. Single-member clusters (54 occurred) are represented by the very small open circles scattered around the other clusters and are regarded as relatively atypical or unique chemically. These relatively rare lake types can be aggregated into the existing clusters for completeness, if desired, but the resulting clusters lose compactness.

The nature of the clusters plotted in Figure 2 may be described from intracluster averages of the clustering variables. Based on the earlier discussion of the sensitivity and response of lake waters to acid and base addition, three clusters of high interest for TIME Project monitoring include Clusters B (Membership=N=166), D (N=18), and G (N=33). The other clusters also are likely to be of interest to ensure representation of major lake types or for other reasons. For illustrating the approach, however, this discussion will focus on Clusters B, D, and G.

The three clusters of interest contain lakes with very similar concentrations of divalent cations (Ca + Mg); however, they are dissimilar in several other respects. As seen in Figure 2, Cluster D lakes were markedly reduced in bicarbonate ion, compared to Clusters B and C. Further, lakes in Cluster D had an arithmetic mean pH of 4.82, compared with 6.85 and 6.75 in Clusters B and G, respectively. Organic acids influenced these differing levels of acidity, as average DOC in Cluster D (4.7 mg/L) exceeded that of Clusters B and G by three- and tenfold, respectively. Much of the acidity difference, however, was due to elevated mean sulfate ion concentration in the highly acidic Cluster D lakes (113.4 ueq/L). Clusters B and G averaged 6.2 and 19.5 ueq/L for this parameter. From these comparisons, it seems reasonable to suspect that the Cluster D lakes, all of which are situated in the northeastern United States, have experienced significant replacement of bicarbonate by sulfate ions, possibly attributable to atmospheric sources.

Cluster D lakes averaged approximately twofold greater conductivity levels compared to those in the other two clusters (23.6 versus 8.3 and 9.5 uS). This difference, however, was due largely to high concentrations of sulfate ion and extractable Al (165.1 ug/L versus 5.8 and 4.4 ug/L) in the highly acidic Cluster D lakes, rather than to road salt contamination or other watershed disturbance. Chloride levels in lakes of the three clusters were very low, and averaged less than 15 ueq/L, which suggests little direct watershed disturbance in these lakes.

The largest contrast between lakes in Clusters B and G occurred with sulfate and nitrate ion concentrations. Lakes in Cluster G contained mean sulfate and nitrate ion concentrations of 19.5 and 4.0 ueq/L compared with 6.2 and 0.9 ueq/L for Cluster B lakes. Inasmuch as both Cluster B and Cluster G lakes were located exclusively in the western United States and both contained lakes from all western subregions, these differences may not be attributable to regionally distinct patterns in SO_4 deposition.

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Non-Parametric Clustering of Drainage Lakes
National Lake Survey Regions 1 and 4

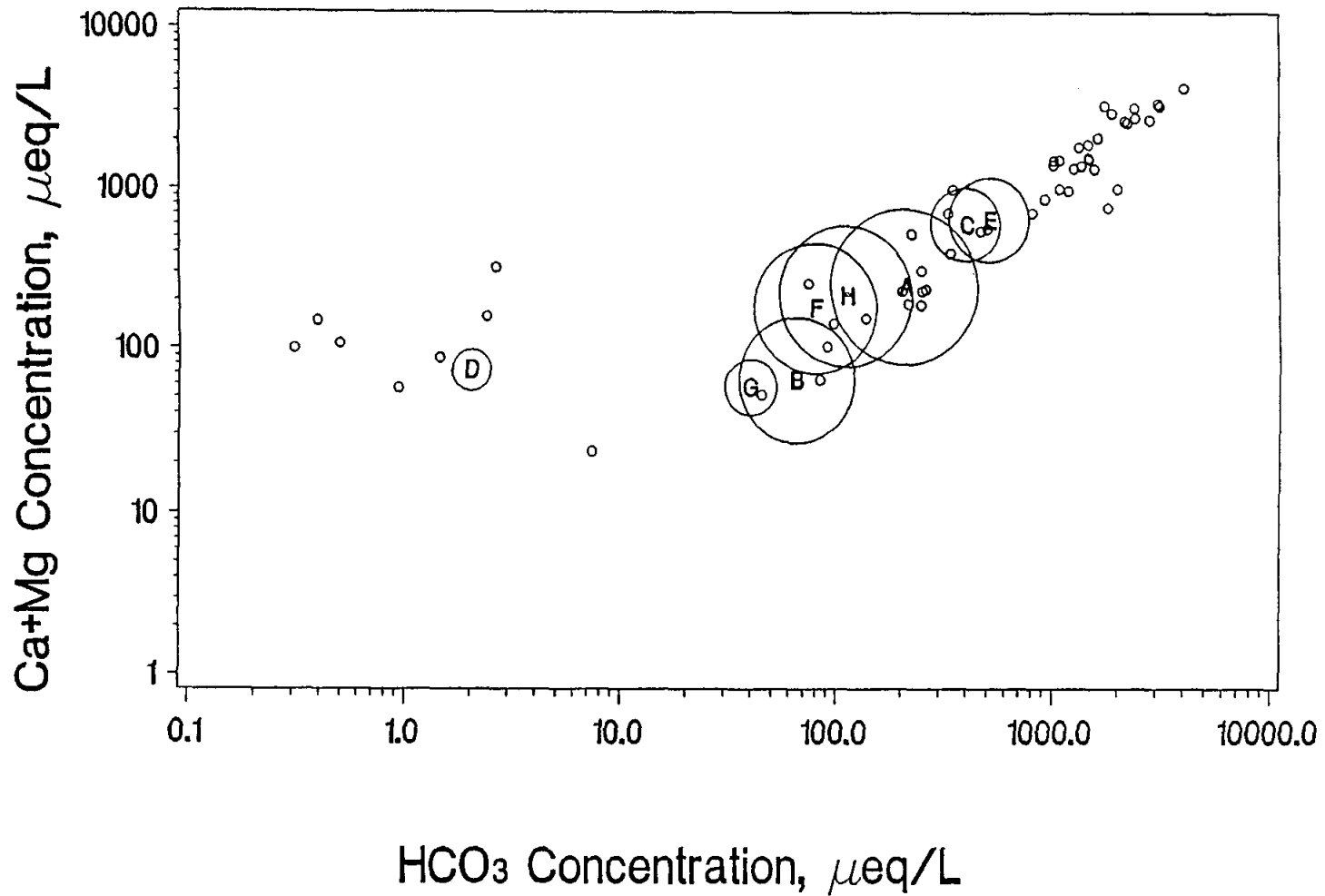**HCO₃ Concentration, μeq/L**

Figure 2.   Ordination of drainage lake clusters on base cation --bicarbonate anion

concentration axes; clusters formed from lakes shown in Figure 1.

To draw a sample of lakes for monitoring from these clusters, cluster membership can be treated as a class variable, and a stratified sample may be selected, randomly if desired. Allocation of samples among the clusters may be arbitrary, equal, proportional, or dependent on attribute or cluster variances. The choice of allocation strategies also will depend on available resources, or desired total sample size and the kinds of estimates required of the sample data.

SUMMARY

The TIME Project requires water quality monitoring in lakes and streams to allow (1) early detection of aquatic ecosystem responses to acidic deposition, (2) assessment of regional patterns and trends in surface water acidity status, (3) verification of watershed model forecasts of water quality response to atmo- spheric deposition, and (4) evaluation of the correlation between surface water quality and atmospheric deposition. To achieve these objectives, various monitoring site selection approaches will be required. This paper has touched on several and explored one approach that makes use of data from lakes sampled during the NLS. The method provides a sample of lakes that is appropriate to the objective of early detection of ecosystem response.

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ESTIMATION OF WET DEPOSITION TO SURFACE WATER SYSTEMS FOR THE TIME PROJECT: A GEOGRAPHIC APPROACH

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INTRODUCTION

One of the major goals of the TIME project is to assess relationships between trends in water quality and trends in deposition (see Pollack and Ford, this issue, for a complete discussion of TIME goals). To realize this goal, accurate estimates of wet deposition to surface water systems are needed. At present, the majority of measurements of wet deposition available for use in this study come from the National Acid Deposition Program/National Trends Network (NADP/NTN) (Olsen, 1988). NADP/NTN deposition monitors are sparsely located, and there is some question as to the whether these monitors can adequately represent wet deposition to trend (early warning) water systems and regions of interest (as represented by regional probability samples of water systems). Specifically, the questions are:

- Given a trend (early warning) water system, can wet deposition of major ions to that system be adequately represented by data from existing monitoring sites?

- Given the existing monitoring sites in a region, can wet deposition to the region be adequately described by these monitors?

Three main research tasks have developed from our efforts to address these questions and insure that adequate monitoring data are available:

(1) Review of factors contributing to the spatial and temporal variability in wet deposition. (What types of variability are we likely to encounter when we monitor wet deposition?)

(2) Development of methods to optimize the usefulness of data from existing networks. (How do we make the most of what we have?)

(3) Development of a wet deposition monitoring network that meets the needs of the TIME program. (What are the criteria that make a network "good enough?" How do we develop a monitoring network that meets these criteria?)

The work to date has been primarily on tasks 1 and 2; methods to deal with task 3 are still being developed. In task 1 we seek to identify those factors that are expected to be important determinants of spatial and temporal patterns in wet deposition. In task 2 we develop methods to make the best possible deposition estimates using available data and knowledge of the factors identified in task 1. The estimation method currently under development is termed Subregional Interpolation (SI), and is dicussed in detail in a later section. Task 2 is of major importance, because optimizing the usefulness of existing monitors reduces the need for adding new monitoring sites to the network (which is an expensive prospect). Task 3 is the ultimate goal of this effort - to develop a

monitoring network that will meet the needs of the TIME project. This requires that we be able to quantitatively compare the uncertainty associated with a deposition estimate with the "tolerable" uncertainty specified by project goals, and gauge the incremental improvement in accuracy achieved by adding monitoring sites to the network. This paper summarizes work in progress in tasks 1 and 2, and concludes with an approach for pursuing task 3.

FACTORS CONTRIBUTING TO THE SPATIAL AND TEMPORAL VARIABILITY IN WET DEPOSITION

Spatial and temporal patterns of wet deposition are undoubtedly influenced by a variety of factors, depending on the geographic characteristics of the site or region of interest and the time and space scales involved. Few field analyses are available on which to base a rigorous evaluation of the factors influencing the variability in wet deposition, but we can supplement the field results with simple theoretical arguments to speculate on the more important factors involved.

In general, the more geographically complex a region and the smaller the time and space scales involved, the more factors are apt to play major roles in determining wet deposition patterns. For example, in regions of the United States where terrain features are minimal (e.g., the Great Plains), spatial patterns of annual wet deposition are probably influenced primarily by factors such as pre- cursor emission patterns and large scale air flow trajectories. However, in geographically complex regions (e.g., the western United States), annual deposition patterns are strongly influenced by the interplay of elevational and topographic effects in addition to precursor emission patterns and large scale air flow trajectories, among others. If the time scale of interest is reduced from a year to, say, a season, seasonal variations in parameters such as rates of atmospheric chemical reactions and storm patterns would tend to play increasingly greater roles in determining patterns of deposition. Decreasing the spatial scale from a large region of the United States down to a particular watershed may bring into play a

host of topographic factors that were insignificant on a regional scale.

Two sets of time and space scales are of interest in the TIME project. The intended water quality sampling interval for the trend water systems is monthly or seasonal, so wet deposition estimates at the watershed level are required at seasonal or monthly intervals. Regional estimates of wet deposition at annual intervals are sufficient for the regional water systems, because water quality sampling will probably occur at an interval of no less than two years. As discussed above, patterns in wet deposition typically become more complex as the spatial and temporal scales are reduced. Hence, the estimation of wet deposition at the watershed spatial scale and monthly or seasonal temporal scale presents the greatest .challenge, and is given the most attention in this paper. Below is a discussion of the more important factors that can influence the spatial and temporal variability in wet deposition. To conserve space, only a qualitative discussion of these factors is included; papers containing quantitative data and analyses are cited where relevant.

Spatial Variability

Most factors influencing the spatial variability in wet deposition fall into four main categories: emission and transport patterns, elevational factors, topographic factors, and proximity to water bodies. The emission and transport patterns of acidic and alkaline pollutants and precursors (sulfur oxides, nitrogen oxides, ammonia, etc.) have obvious effects on the spatial variability in wet deposition. Barring variations in precipitation amount, sites that are downwind and in close proximity to major emission sources will typically experience higher concentrations in precipitation than sites upwind and distant from major emission sources.

Changes in elevation may cause variability in wet deposition as a result of changes in (1) precipitation amount (which affects wet flux); (2) precipitation type (e.g., rain vs snow, which affects scavenging processes); and (3) vertical mixing of polluted air with clean air aloft (which tends to decrease concentrations

at high elevations). The relationship between elevation and precipitation amount is probably the most important factor in this category. In the western United States, precipitation amount is affected strongly by orographic effects; as a result, precipitation amount is strongly elevation-dependent (Corbett, 1967). While orographic effects exist in other parts of the country, they are often subtle and can be more difficult to quantify (e.g., Johannes and Altwicker, 1986). Differences in precipitation type and accompanying scavenging mechanisms have been suggested as reasons for variations in the nitrate/sulfate ratio during winter (e.g., Altwicker et al., 1986), but the processes involved are not well understood. Vertical mixing of polluted air with clean air at upper levels in the atmosphere is also poorly understood, but may be important at high elevations (Daly et al., 1989a).

Topographic factors influencing the spatial patterns of wet deposition include (1) slope exposure (leeward vs windward) and steepness; and (2) separation by hills and ridges. Sites on windward slopes are exposed to upwind pollutant sources and are probably located in areas of orographic lifting and condensation; hence, wet deposition would be relatively high. In contrast, sites on leeward slopes would be largely cut off from upwind pollution and moisture sources, resulting in relatively low wet deposition. Slope exposure effects tend to become amplified when the steepness of a a slope is increased (Pagnotti and Rao, 1986). Sites separated by hills and ridges may experience air flow trajectories that have different origins, because of channeling and upslope/downslope flow processes; this may cause the sites to be affected by different emission source areas.

Large water bodies such as oceans and the Great Lakes influence the spatial variability in deposition by acting as sources of moisture (which affects precipitation patterns) and sources of certain ions and compounds (which affects concentration patterns). A classic example of a lake acting as a moisture source is "lake effect" snowfalls on the southern shore of Lake Erie, caused by the entrainment of the lake's moisture into cold, continental air advecting across its surface. The oceans

are a well known source of ions in precipitation (Junge and Werby, 1958; Granat 1972). The entrainment of sea spray into the atmosphere produces elevated concentrations of chloride, potassium, calcium, magnesium, sulfate, and sodium at coastal sites.

Temporal Variability

Factors contributing to the temporal variability in wet deposition can be grouped by their associated time scales: event-to-event factors, seasonal factors, and annual factors. Event-to-event factors deal primarily with the characteristics of a storm system that produces a precipitation event. Such factors include storm type (e.g., frontal type and wind field configuration), storm path relative to the site (e.g., what sector(s) of frontal system affects the site) and storm intensity (e.g., rainfall amounts and wind speeds). Storm characteristics can vary widely from event to event, producing highly variable time series of event-based deposition at a site.

Seasonal variability in wet deposition is largely due to variability in (1) dominant storm patterns; (2) solar radiation (affecting the rate of chemical reactions in the atmosphere), (3) dominant precipitation type (rain vs. snow), and (4) emission rates and patterns. Certain seasons of the year are associated with "typical" storm patterns. For example, precipitation events over much of the southeastern United States are caused primarily by frontal systems during winter and air mass thunderstorms during summer; each pattern is characterized by typical emsisions trajectories and precipitation patterns.

Ultraviolet radiation from the sun drives chemical reactions in the atmosphere that produce oxidants and convert precursors into acidic compounds; changes in the incident solar radiation produce changes in reaction rates. For example, a common chemical pathway in the formation of acidic sulfate is a reaction of sulfur dioxide with hydrogen peroxide in the aqueous phase; hydrogen peroxide is formed in the presence of sunlight. It is not suprising, then, that seasonal concentrations of sulfate in

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precipitation typically peak during the summer months.

In the northern portion of the United States and at high elevations snow is the dominant precipitation form during winter; spring and fall are characterized by a mix of rain and snow events, and summer is dominated by rain. Differences in scavenging mechanisms between rain and snow events may favor one pollutant over another, resulting in seasonal biases in the concentrations of pollutants in precipitation (Altwicker et al, 1986). As mentioned previously, this factor is not well understood and may be difficult to isolate.

Some emission sources exhibit a significant seasonal variability; such sources include automobile traffic, residential fuel combustion, agricultural activities, and biogenic emission sources (e.g., emissions of hydrocarbons from vegetation) (Wagner et al., 1986). Since different emission sources may exhibit different seasonal variabilities, both the patterns and magnitudes of emissions, and hence, deposition, may change from season to season.

Annual variability in wet deposition is due primarily to variability in climatology and emissions (e.g., Granat, 1975; Munn et al., 1984; Likens et al., 1984). Each year is different climatologically; annual frequency distributions of storm type, path, and intensity from adjacent years are rarely identical. Emission source strengths and patterns vary as a result of emission controls, changes in operating capacity, and the construction of new and elimination of old sources.

Overall, it appears that event-to-event factors will not be of direct concern to the TIME project. The major factors influencing the temporal patterns of wet deposition will probably be those at the seasonal and annual time scales. For estimating wet deposition to trend water systems, dominant storm patterns and atmospheric chemistry appear to be of greatest overall importance. For estimating wet deposition to regionally sampled water systems, only annual factors need be considered. Both climotological and emissions

trends are important factors in the interannual variability of wet deposition.

OPTIMIZING THE USEFULNESS OF EXISTING DATA

Armed with information on the potential variability in wet deposition and educated guesses as to the factors involved in this variability, we can consider methods by which existing data can be best interpolated or extrapolated to represent deposition to watersheds and regions. In general, there are two types of methods presently in use: quantitative methods and qualitative methods. Quantitative methods consist mainly of objective, numerical approaches to data interpolation. Kriging and $1/r^n$ distance weighting are popular quantitative approaches to estimating wet deposition. Kriging, a geostatistical estimation technique, involves the development of semi-variogram functions to describe the spatial variability of the parameter of interest combined with an estimation technique that minimizes the variance of estimation errors. Because the method relies on an empirically-derived semi-variogram function, extrapolation of data into regions outside the coverage of the semi-variogram (i.e., "corners" of a region where no data exist) may not be feasible unless a background or average value is specified along the edges of the domain. Good discussions of kriging can be found in Finkelstein (1984); Seilkop (1986); Guertin et al., (1989); and Vong et al., (1989). Kriging is not an entirely objective approach, because there is subjectivity involved in choosing a semi-variogram model (Vong et al., 1989). Kriging is currently the preferred choice for the estimation of wet deposition because the method provides effects researchers with an estimate of the estimation error involved.

The $1/r^n$ approach weights the influence of data points by their distance (r) from the estimation point. The weighting curve depends on the specification of the exponent n, which is typically set at 2 or 3. The greater the value of n, the more a distant data point will be downweighted relative to a nearby data point. Uncertainty estimates are not routinely provided when the $1/r^n$ method

is used. Vong et al. (1989) point out that uncertainty estimates can be made for the $1/r^n$ method (e.g., using cross-validation or the construction of an equivalent semi-variogram model), but are not routinely incorporated into software containing the technique. By using a preset distance weighting function, the $1/r^n$ method can extrapolate a parameter into regions of a domain where no data exist.

Qualitative approaches to interpolation involve "eyeballing" spatial patterns and hand-drawing maps of the parameter of interest. In the case of wet deposition, the approach uses human expertise to combine knowledge of emissions sources, climatology, air chemistry, and geography to accurately model the spatial patterns in the data. It is acknowlegded, however, that different analysts will produce different maps for a given data set (Vong et al., 1989).

Overall, both types of interpolation methods have advantages and disadvantages. Most quantitative methods are objective, repeatible, and transportable (can be easily applied to other problems); some methods, such as kriging, can give estimates of the uncertainties in the interpolated data fields. While they are of great use in situations where data are plentiful, they may give physically unrealistic results when used in data-sparse situations. The methods are, in essence, "blind" to the physical factors that cause spatial variability in wet deposition; the methods rely on the deposition data to reflect the influences of these factors. Qualitative methods, on the other hand, rely on the broad knowledge and intuition of the analyst. If the analyst is skilled, he or she can supplement a sparse data set with additional data and personal knowledge to produce contour maps that have more physical meaning than quantitatively-produced fields. However, the method introduces personal biases of unknown magnitude and cannot be easily repeated (e.g., by different analysts). The expertise required for a qualitative analysis is particular to the problem at hand and changes as the geographic region or the parameter to be interpolated changes; the method is therefore not universal or portable. In addition, the uncertainty of the interpolated data field is unknown, so it is impos-

sible to judge whether an interpolated field is sufficiently accurate for a given application.

## The Subregional Interpolation (SI) Method

It appears that the best method by which estimates of wet deposition can be made should reflect an optimal balance between quantitative and qualitative methods. The optimal method would employ quantitative interpolation tools, but allowances would be made for subjective (but systematic) intervention, such as the use of supplementary data, to interpret the data to its fullest and insure the most accurate and physically meaningful results. The interpolation method currently under development for the TIME project, called Subregional Interpolation (SI), strives to achieve this balance.

The Subregional Interpolation method is based on the concept that interpolation error can be reduced substantially by dividing a region into geographically-based subregions within which the parameter of interest behaves similarly spatially and temporally (i.e., is affected by similar factors). Figure 1 presents a simplified illustration of this concept. Suppose we wish to estimate wet deposition to the lake shown in Figure 1a. Of the two monitors in the area, the one to the north of the lake is twice as far from the lake than the one to the west. If we apply a distance-weighted interpolation scheme to this problem, we would expect interpolated wet deposition at the lake to resemble measurements at the monitor to the west. (And at this point we would have no reason to disagree with the result.)

Let us consider the same problem, but from the perspective of Figure 1b, for which some geographic information has been added. Now, the problem can be restated as follows: suppose we wish to estimate deposition to a high-elevation lake on the lee side of a mountain range. There are two wet deposition monitors in the area -- the closest is on the windward side of the range and at low elevation, while the farthest is on the same side of the range and closer to the crest of the range. Emission sources are some distance upwind and out of the figure. Our distance-weighted interpolation scheme cannot
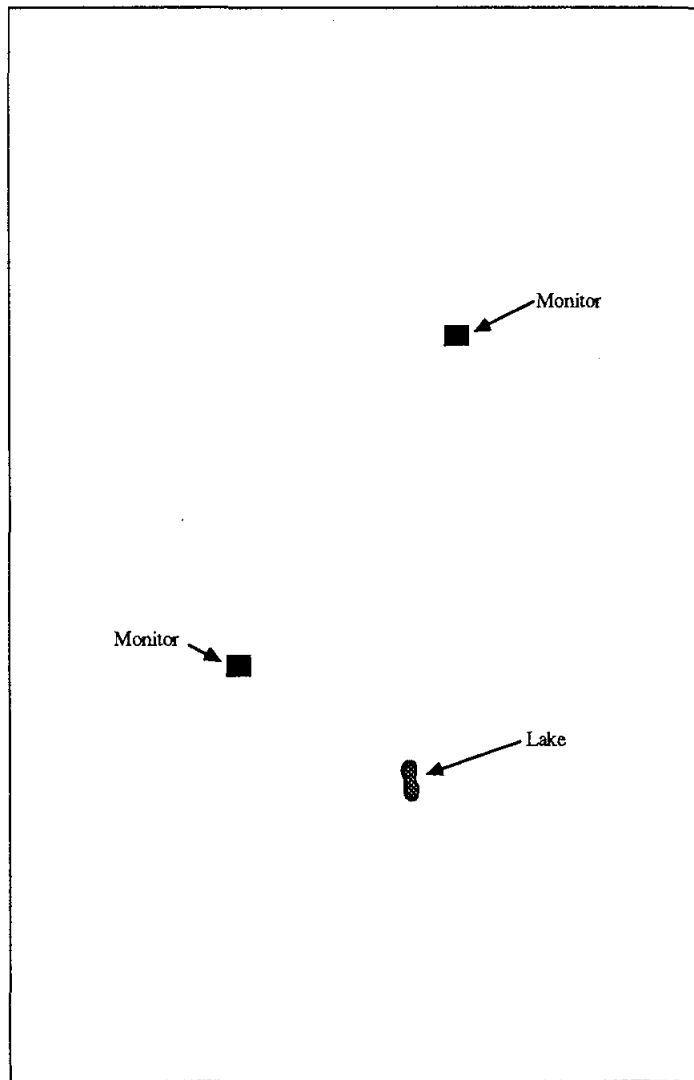
(a) View as Seen by an Objective Interpolation Algorithm
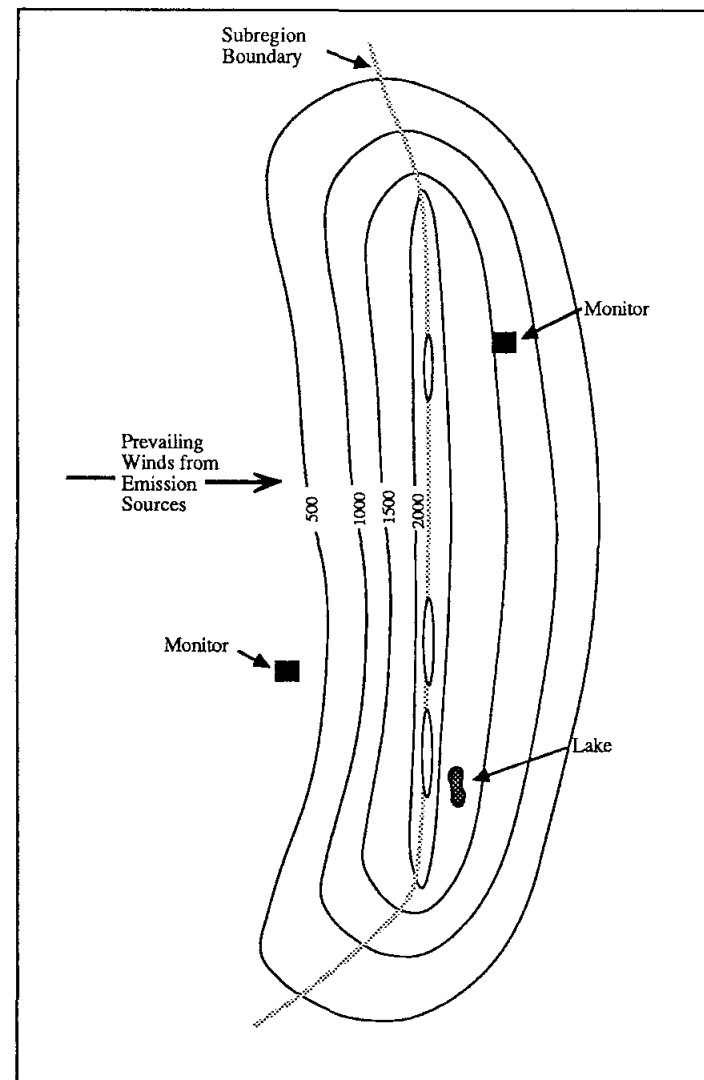
(b) View from a Geographic Approach

FIGURE 1.   Suppose we wish to interpolate deposition to a lake from two monitors. Figure (a) gives information required by a distance-weighted interpolation scheme. Figure (b) provides additional geographic information, which significantly increases our understanding of the problem.

consider this new information, and would produce the same result as before. However, this result now appears unrealistic. Simple information on emission source location, topography, elevation and wind direction suggests that the leeward, distant monitor would be more representative of the lake than the windward, nearby monitor. An effective way to numerically "advise" the interpolation scheme of this situation is to divide the area into two subregions, a windward subregion and a leeward subregion, and exclude the windward monitor from the estimation of deposition to the leeward lake (Figure 1b).

The Subregional Interpolation method has been recently developed and successfully applied to mesoscale air quality modeling studies, for which highly resolved fields of meteorological data (e.g., temperature, depth of atmospheric mixing) are required for model input. The SI method performed extremely well in modeling studies in the San Francisco Bay Area and Santa Barbara-Ventura County area, where traditional applications of objective interpolation techniques (i.e., kriging and $1/r^n$ inverse-distance weighting) failed to simulate large gradients in meteorological parameters produced by complex terrain and coastal influences (Daly, 1989b, 1989c; Moore, 1989). Typically, the regions were divided into subregions such as "ocean," "coastal strip," "coastal valleys," and "inland highlands," in which the parameter of interest was affected by similar factors. Interpolation, using $1/r^2$ or kriging, then proceeded within each subregion separately.

In general, the SI method consists of four main steps:

(1) Using both quantitative and qualitative data and analysis methods, delineate geographic subregions within which the parameter of interest behaves similarly, spatially and temporally.

(2) Within each subregion, develop quantitative relationships (if possible) between the parameter of interest and influencing factors (e.g., elevation, distance from emission sources).

(3) Interpolate the parameter to a grid within each individual subregion.

(4) Apply a smoothing algorithm (e.g., a five- or nine-point filter) to minimize discontinuities between subregions.

The careful delineation of subregional boundaries is the key to the SI method, and the most difficult step. Choosing subregional boundaries requires thoughtful, informed consideration of many kinds of data, both qualitative and quantitative. Qualitatively, maps depicting spatial patterns of deposition and potential influencing factors should be prepared or obtained. These maps should include (1) rates and locations of relevant emissions (e.g., NAPAP 1985 gridded inventory of NO_x, SO_x, and NH_3); (2) topogaphy, including elevation; (3) prevailing wind directions and flow patterns; (4) climatological regions (e.g., those prepared by state climatologists); (5) station measurements (uninterpolated) of monthly and annually averaged concentration and deposition of major ions; and (6) station measurements (uninterpolated) of monthly and annually averaged precipitation.

Quantitatively, for example, correlation analyses of deposition and concentration between pairs of existing monitors can be performed. Questions to ask might be: is there a gradual decrease in correlation between monitors as distance increases, or are there obvious "break points" that may suggest subregion boundaries? Are there certain pairs of monitors that, while in close proximity, exhibit unusually poor correlation? They may be straddling a subregion boundary. Are all sites poorly correlated? This would indicate that each monitor probably belongs in a separate subregion, and that the network is insufficient to help delineate subregions.

More sophisticated approaches might include applications of clustering or splitting algorithms (a popular splitting algorithm is the Classification and Regression Tree (Breiman et al., 1984)). These analysis can be supplemented with variables other than those directly related to deposition. For

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example, station data on deposition of various ions, elevation, topographic exposure, and distance from water bodies could be input for each station, and the stations grouped into clusters that have similar geographic, as well as deposition, characteristics; these clusters may then be suggestive of subregional groupings.

Similar analyses could be conducted for precipitation gauge data, which is more plentiful than concentration data. However, those factors influencing precipitation patterns may be different than those influencing concentration patterns. Questions concerning the usefulness of the indirect method of interpolating deposition (where precipitation data are used to achieve greater spatial resolution in the deposition field) should be asked here (e.g., Wampler and Olsen, 1987).

Efforts to delineate subregional boundaries should always be oriented towards the development of a rule-based system that codifys at least some of the major decisions made in the delineation process. This may involve the development of an expert system that can follow a prescribed decision tree. The more objective the process, the more the process can be treated as quantitative, with the accompanying benefits (e.g., transportable, repeatable, etc.).

A subregion need not be a single polygon, but can exist in several "pieces." This situation occurred often in our application of the SI method to temperature interpolation for coastal modeling regions. For example, a series of coastal valleys extending from the ocean into mountainous terrain possessed the same temperature characteristics, but were separated from each other by higher terrain. Under the SI method, each valley was included in the "coastal valleys" subregion and each intervening mountain area was included in the "coastal mountains" subregion. An advantage to this feature is that in cases where data are sparse, a monitered value in one area can be used to represent other areas some distance away that are in the same subregion.

Within the subregions relationships between physical factors and wet deposition or concentration may be developed or inferred to aid in the extrapolation of data points, if data are sufficient. For example, it may be possible to develop regressions between precipitation and elevation. By definition, relationships between influencing factors and deposition (or its components, concentration and precipitation) should be relatively strong within subregions, if they are delineated accurately. The largest obstacle will be the availability of data from which to develop the relationships.

The interpolation of deposition within each subregion requires specifying a grid and applying the intepolation scheme. Ideally, subregions would be superimposed onto a master grid that incorporates the entire region of interest. The appropriate size of a grid cell would depend on the spatial scale of interest, geographic complexity, and the subregion size. The interpolation method should be numerical and objective, and be supplemented by relationships between deposition and physical factors that were developed for the subregion. The indirect method of estimating deposition (i.e., using precipitation data to increase the spatial resolution of the deposition fields) should be considered for use wherever valid.

Lack of inter-subregional influence during the SI process gives the interpolated data field the look of a jigsaw puzzle, with sharp gradients along the edges of the "pieces," or subregions. Theoretically, this is not a totally unwanted result; subregion boundaries are supposed to denote boundaries between areas that exhibit differing behavior with respect to wet deposition. However, in reality there will be a certain amount of crosstalk along the edges of the subregions that will blur these sharp transitions. Spatial filters can be applied to the interpolated field to simulate this smoothing process. The typical filter used in previous applications is a five- or nine-point filter designed to minimize or eliminate spatial variations with wavelengths of two grid cells.

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Difficulties in Applying the SI Method to the TIME Project

We are currently grappling with a difficult question concerning a peculiar aspect of applying the SI method to the TIME project: since a region can be subdivided an unlimited number of times, down to the watershed level, how do we know when to stop the subdivision process? In previous applications of the SI method, the answer was relatively simple: do not create subregions that have no data to represent them. Unfortunately, the application to the TIME project is different; we must be able to recommend additional monitoring sites, if needed, to develop a network that will be sufficient for the needs of TIME. An ideal way to show a need for monitors is to point to subregions with no monitors representing them!

In theory, the subdivision limit should be the point at which the uncertainty of the interpolated field becomes less than the "tolerable" uncertainty of the TIME analyses (a major issue in task 3). One way to estimate the uncertainty of the interpolated field within subregions is to use the "close" end of the semi-variogram used in kriging to examine small-scale variances. This would be best used when there is at least one monitor per subregion (i.e., before unmonitored subregions are delineated). However, the lack of data within a subregion would require that we make the assumption that small-scale variances are similar among subregions. Another way to approach the problem is to use correlation analysis to calculate the sphere of influence (SOI) for each station. In this context, the SOI is defined as the surrounding area over which the monitoring station can be considered to be representative, with known confidence (Liu et al., 1986). However, a spatial model of the variability of deposition around each monitor must be constructed to calculate the SOI; the SOI will change as the model changes.

In the end, practical constraints will probably play a large role in determining the subdivision limit, e.g., lack of information on which to base subregion delineations, and the expense of installing a dense monitoring network.

FURTHER WORK: MEETING THE NEEDS OF THE TIME PROJECT

The next step in developing a deposition monitoring network that meets the needs of the TIME project is to begin testing and refining the Subregional Interpolation method of optimizing existing data. A pilot analysis should be initiated in which the method is applied to a region of interest to the project, such as New England or the Adirondacks. If the SI method appears to be feasible, the procedure should be refined and improved. Attempts should be made to develop objective rules for specifying subregions that may be transferred to other regions. Also, it is important to evaluate the method and show that it has advantages over qualitative and quantitative methods alone; this is probably best done through direct comparison with other methods and with observations.

The pilot study should continue with preliminary comparisons of trends in water quality and interpolated deposition. Water quality data from the Long Term Monitoring of Lakes project (LTMP) project (e.g., Newell et al., 1987) can be used as a surrogate for trend site water quality data. Statistical tests, including tests to assess the benefits of indirect estimation of deposition and to assess incremental improvements in data utility by adding monitors, should be developed and tested. Much can be learned from this exercise concerning uncertainties in the water quality and wet deposition data that will help us address task 3 of this work. In addition, problems that may be encountered when analyzing actual TIME trend systems can be anticipated and addressed.

Drawing on all previous analyses, we should then be able to begin to quantitatively assess the representativeness of a wet deposition monitoring network and make recommendations as to what will be required to produce a network that will meet the needs of the TIME project.

Acknowledgements

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WHAT CAN BIOLOGICAL MONITORING TELL US ABOUT THE ENVIRONMENTAL HEALTH OF AQUATIC ECOSYSTEMS?

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INTRODUCTION

Millions of dollars per year are spent on aquatic ecosystem monitoring directed toward these objectives:

- Assess status and trends
- Identify problems
- Refine standards, permits, and best management plans
- Evaluate the effectiveness of management programs
- Set management priorities

In the United States, however, we cannot yet meet even the first objective in any comprehensive manner. Consequently, management programs and priorities for aquatic ecosystems may or may not be fulfilling the Clean Water Act objective "to restore and maintain the chemical, physical, and biological integrity of the Nation's waters."

During this meeting, many speakers expressed similar concerns about monitoring programs.

- What are the biological effects of highly dilute chemical concentrations? (Grigg, this volume)

- What is the current quality of the Nation's waters?

- Why do decision makers make such little use of monitoring information? (Moss, this volume)

- What are we getting for the $80 million we spend yearly on monitoring and pollution control?

- How does the quality of most waters compare with that of more natural environments?

- What are the likely ecological consequences of a management action, or continued inaction?

- If we meet permit and best management plan requirements, has ecological quality been achieved?

- Are we protecting the ability of ecosystems to recover from stress? (Messer, this volume)

- What are our major environmental problems and their probable causes? Are conditions improving, worsening, or relatively constant? (Magnien, this volume)

I contend that a major reason we have difficulty answering these questions is because we frequently monitor the wrong variables, or we monitor or analyze proper variables in wrong ways. The basic questions we must ask are, "How can we best assess the health of entire ecosystems and how can we extrapolate from a limited amount of site-specific monitoring?" Although measurement of standard chemical water quality variables seems to be the preferred approach, there are

several reasons to favor biological monitoring, though not to the exclusion of chemical/toxicological and physical monitoring. In addition, probabilistic sampling and eco-regional based standards offer a means to extrapolate site-specific monitoring data to large regions with known statistical confidence.

VALUES OF BIOLOGICAL MONITORING

Biological monitoring and analysis have advanced considerably in recent times. Historically, biological monitoring focused on indicator species, species presence/absence, or species lists unintelligible to nonexperts. Field sampling lacked rigorous, consistent proced- ures and occasionally involved expensive surveys of all biota over several seasons or. years. Data analyses were simplistic and emphasized post facto "best professional judgement." In this paper, biological monitoring (biomonitoring) is defined as "the collection of quantitative or semiquantitative biological community data at regular intervals and with an established quality assurance (QA) protocol." Recently, the U.S. EPA (U.S. EPA 1987, Whittier 1988, Plafkin et al. 1989, U.S. EPA 1989) has shown increased interest in biological monitoring.

There are eight major reasons for adopting biological monitoring:

1. The biota are of direct concern to the public and to decision makers--many people care about particular game or rare species and about the richness of the biological community in general.

2. Biological monitoring allows assessment of a wide range of stressors--physical, chemical, biological, point, nonpoint, toxic, and nontoxic. It provides a firm basis for assessing nonchemical and nontoxic degradation, which is missing from chemical and toxicological monitoring.

3. Biomonitoring offers a mechanism for evaluating episodic events. The long-term effects of droughts, floods, spills, process changes,and illegal dumping are monitored continuously by organisms.

Traditional chemical/toxicological monitoring is likely to miss such events.

4. The cumulative effects of multiple dischargers and stressors can be examined through monitoring of biological communities. Traditional chemical monitoring misses such synergistic effects.

5. The biota offer a means of estimating (1) bioaccumulation, through chemical analysis of tissues, and (2) indirect effects, through studying the influences of stressors on the food chain, competition, predation, migration, and life histories. These critical community characteristics simply cannot be assessed chemically or physically.

6. Biomonitoring frequently leads to diagnosis of the probable stressor(s) because of the different ways in which different stressors affect various components of the community. For example, comprehensive biological surveys have shown that in many parts of the country physical habitat (structural and hydrological) perturbations and diffuse pollution (particularly clean sediments) are much greater problems than such highly publicized stressors as point sources, acid rain, hazardous waste sites, and toxic chemicals.

7. Biological monitoring provides a direct measure of biological and ecological health or integrity; therefore, it provides a direct measure of whether the objective of the Clean Water Act is being met.

8. Biomonitoring is often more cost effective and less expensive than bioassays and chemical analyses (Table 1), thus it offers a useful screening or problem detection tool.

ADDRESSING ECOLOGICAL VARIABILITY

A basic problem that all environmental monitoring programs must address is ecological variability, both temporal and spatial.

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Table 1. Cost Comparisons for Chemical, Toxicological, and Biological Assessments

Assessment	Number of Samples/Tests	Cost/site ($)
Water Quality	1-6	350-1,700
Bioassay	Grab acute/Composite chronic	3,200-12,600
Macroinvertebrates	1-3	175-700
Fish	1-3	235-900

(From Chris Yoder, pers. comm., Ohio EPA, Columbus, Ohio; Terry Maret, pers. comm., Nebraska Department of Environmental Control, Lincoln, Nebraska).

These are inherently interrelated and often difficult to distinguish. We can assess the magnitude of temporal variability by sampling frequently, but most monitoring programs lack the resources to do so. In ecological assessments, we attempt to minimize the influence of temporal variability in four ways:

1. Sample during periods of relative stability in flow and temperature, when assemblages are most stable and species least likely to migrate; at these times, anthropogenic stressors are less variable and typically most stressful.

2. Sample longer-lived species (e.g., macroinvertebrates and fish in streams and rivers), which are temporally the most stable components of the aquatic biota. Long-lived species are less influenced by daily temperature/flow/ nutrient changes and they integrate longer term influences rather than the short-term fluctuations that can be considered as ecological noise (in a statistical sense).

3. Record the number or biomass of individuals of each species collected for a given unit of effort or area sampled. Such data are generally more informative of status and trends than presence/ absence or rare/common/ abundant data and are much more easily and reliably collected than absolute abundances.

4. Analyze multiple structural and functional characteristics of assemblages as opposed to individual species or a single metric, such as a diversity index. This further reduces natural temporal variability resulting from species replacements that fill the same ecological niche.

Although not complete measures of ecosystem health, these assessments reflect the basic changes in the biota that occur over a single season or over years.

Like temporal variability, spatial variability can be accommodated. Toward this end, scientists at the U.S. EPA Environmental Research Laboratory in Corvallis, Oregon,

have developed and evaluated a means for aquatic scientists and managers to stratify spatial variability. This method, called the ecoregion approach (Omernik 1987, Hughes and Larsen 1988), is a deductive technique based on the natural spatial (geographical) organization of ecosystems. In this approach, the patterns in ecosystem regions are evaluated through analysis of available maps, and ecoregion boundaries are delineated by synthesizing the maps (Figure 1). This is a qualitative technique requiring considerable geographic knowledge and expertise. The basis for this approach is the understanding that the character of a water body (e.g., its water quality, flow regime, habitat structure, energy base, and migration barriers) is in large part a function of the climate, topography, geology, soil, vegetation, and land use of its drainage basin.

Within each ecoregion, a series of minimally impacted reference sites (controls, benchmarks) is monitored (Hughes et al. 1986). Reference sites are selected to be as typical of the natural ecoregion conditions as possible; their selection is based on:

Minimal perceived impacts from stressors common to the ecoregion

Proximity to official and de facto biological refuges

Fewer migration barriers

Water body size and channel or basin type

Evaluation of historical conditions

Candidate sites are located on maps, then reconnoitered at ground level, and from aerial views, if possible. The biota and habitat are then quantitatively sampled and the data analyzed and ranked.

BIOLOGICAL DATA ANALYSES

The assemblages chosen are usually a function of the water body, stressor of concern, and staff expertise; however, the U.S. EPA recommends that more than one assemblage be chosen to account for differing
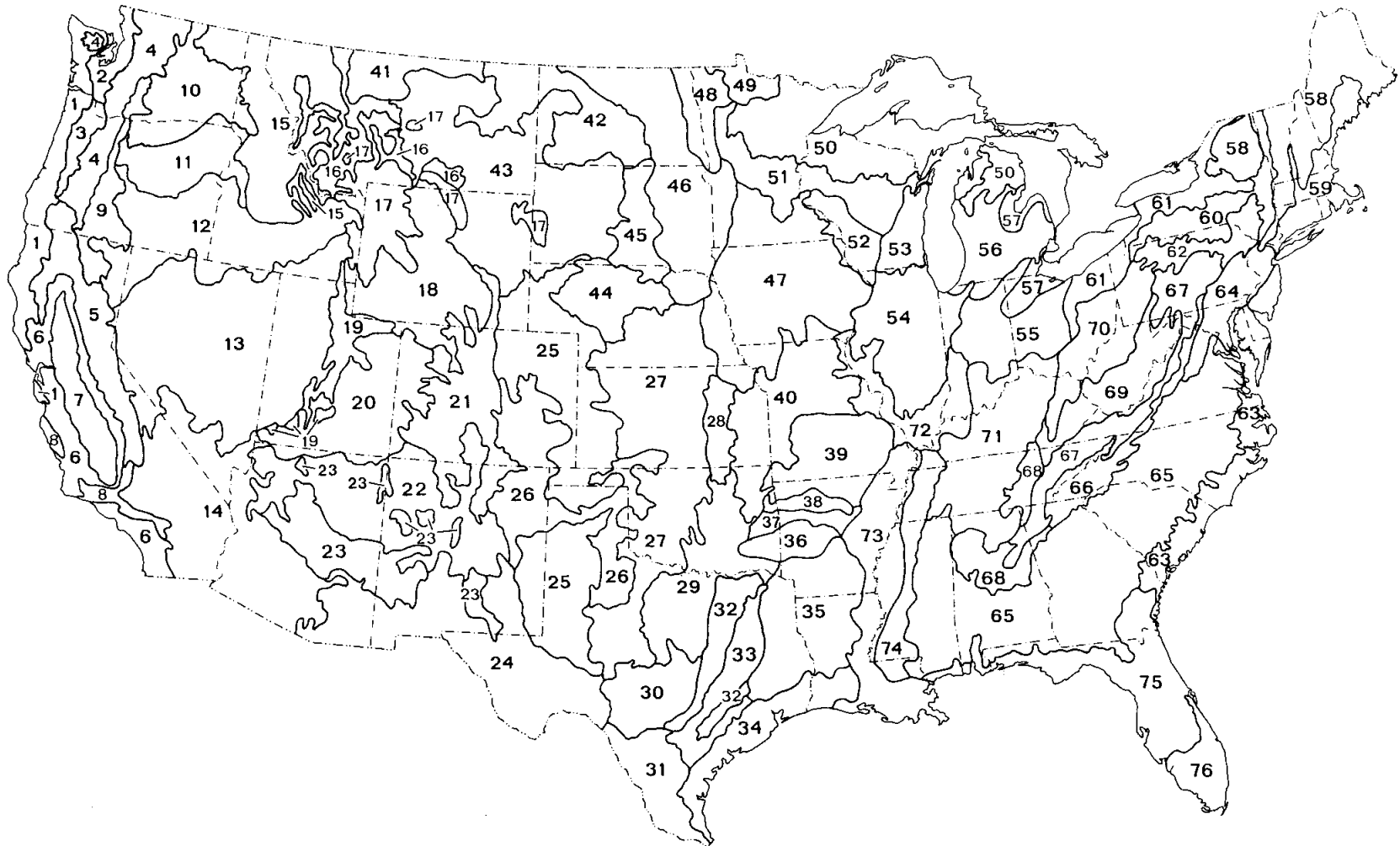
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Figure 1.   Ecoregions of the conterminous United States (from Omernik 1987). Numbers represent
             the 76 different ecoregions. Most major river basins cross ecoregions; therefore, reliable
             basin-wide extrapolations are hindered by drastically different types of landscapes.

sensitivities and provide additional verification (Whittier 1988, Plafkin et al. 1989). Monitoring of all possible assemblages is not recommended. Assemblages to be monitored should be selected carefully, by experienced biologists, to assure sufficient representation of the system but to avoid needless duplication and increased cost.

Histograms and detrended correspondence analyses are particularly effective for displaying ecoregional differences in species assemblages (Whittier et al. 1988; Figures 2 and 3). Indices of assemblage quality, which integrate several measures of biological health, are more useful for assessing and quantifying status, trends, and ecological integrity. One such index, the Index of Biotic Integrity (IBI) (Karr et al. 1986), is a quantification of a fish ecologist's judgment of the relative quality of a fish assemblage. The IBI is composed of 12 metrics (appropriately modified for different regions), each of which measures a different aspect of fish assemblage health (Table 2). Metric values approximating, deviating slightly from, or deviating greatly from expected ecoregional reference site values are scored 5, 3, or 1, respectively. The scores are added to give an IBI score of 60 (excellent) to 12 (very poor).

Quantitative indices such as the IBI and individual IBI metrics offer direct, objective, repeatable measures of aquatic ecosystem health (Karr et al. 1986, Lenat 1988, Ohio EPA 1988, Plafkin et al. 1989). For example, the Ohio EPA (1988) used the IBI and ecoregional reference sites to set quantitative biological criteria for stream and river ecosystems. One hundred regional reference sites were sampled three times a summer during a 2-year period and regional IBI values were determined. Regional criteria, based on the results from these sites, were set at the 25th percentile (Figure 4) and have been used to assess the impact of stressors on a particular river reach (e.g., Figure 5) or statewide (Figure 6). The IBI has also been used to assess site-specific trends over time in aquatic ecosystems (Figure 7).

SUMMARY

Biological monitoring offers a proven, cost-effective way to evaluate the health of aquatic ecosystems. For the sake of brevity, this paper focuses on examples using fish assemblages and the IBI, but fish and macroinvertebrate assemblages provide complementary information and it is best to monitor both for streams and rivers. Macroinvertebrates have been sampled for many years, but only recently have rigorous multimetric indices been suggested for them (Lenat 1988, Ohio EPA 1988, Plafkin et al. 1989), and the indices have not yet been tested as widely as the IBI. Quantitative biological data from relatively undisturbed reference sites typical of aquatic ecoregions provide us with benchmark information, hence these sites serve as "controls" in our "experiments" with anthropogenic perturbations. This information can be used to evaluate data for a particular site or, if a representative sample is drawn, for entire ecoregions. Finally, although this paper focuses on biological monitoring because of the current emphasis on chemical monitoring, it is not meant to suggest that physical habitat and chemical/toxicological monitoring are valueless. Rather, quantitative criteria developed from all three types of monitoring are necessary tools for improved water resource regulation and management (Figure 8).
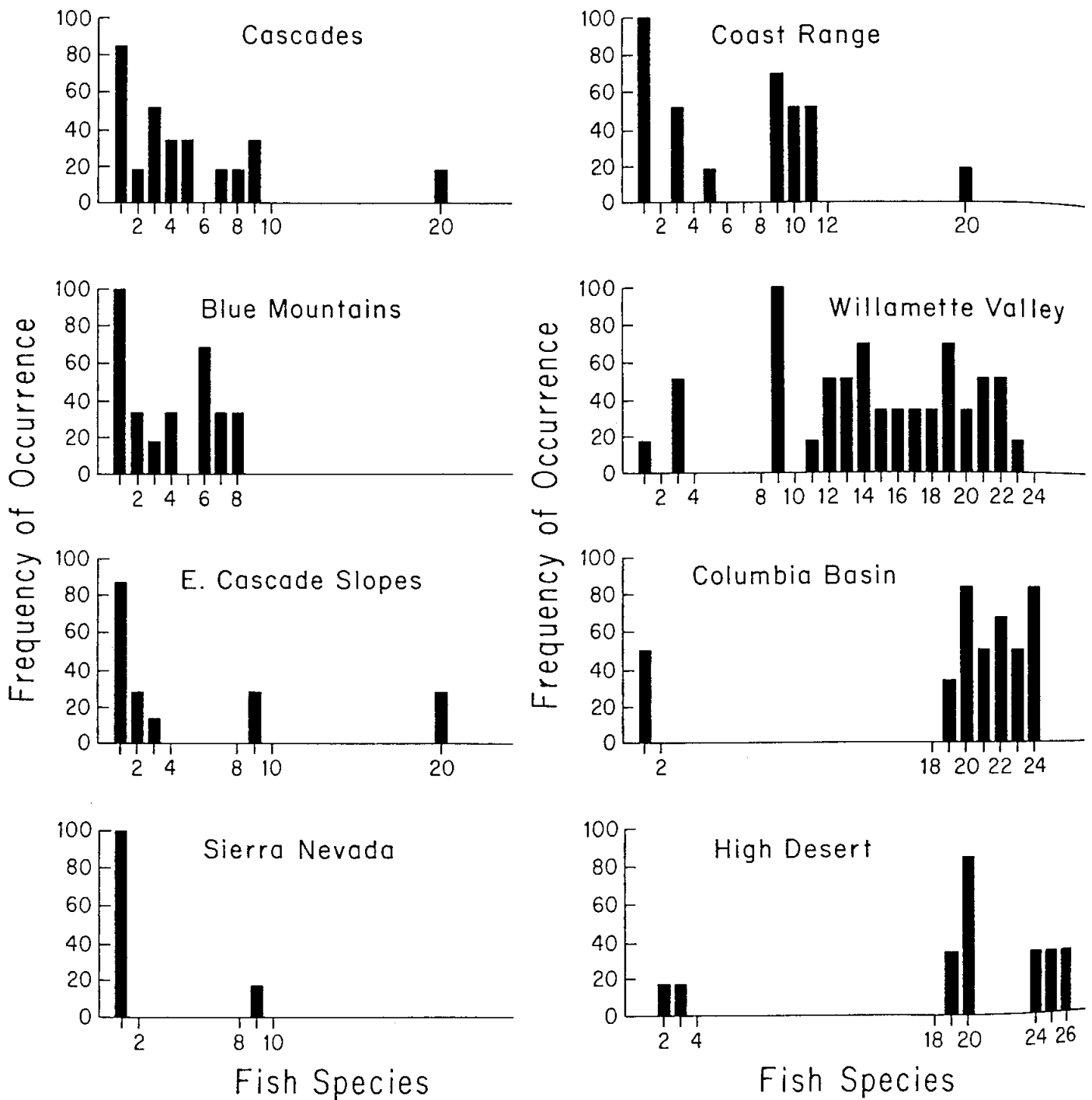
ACKNOWLEDGEMENTS

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Figure 2. Histograms showing frequencies of occurrence of 26 fish species common to Oregon ecoregions (from Whittier et al. 1988). 1. Rainbow trout, 2. Brook trout, 3. Cutthroat trout, 4. Mottled sculpin, 5. Torrent sculpin, 6. Bull trout, 7. Piute sculpin, 8. Mountain whitefish, 9. Reticulate sculpin, 10. Pacific lamprey, 11. Coho salmon, 12. Pacific brook lamprey, 13. Warmouth, 14. Bluegill, 15. Largemouth bass, 16. Common carp, 17. Mosquitofish, 18. Threespine stickleback, 19. Redside shiner, 20. Speckled dace, 21. Largescale sucker, 22. Northern squawfish, 23. Chiselmouth, 24. Bridgelip sucker, 25. Tahoe sucker, 26. Redband trout.
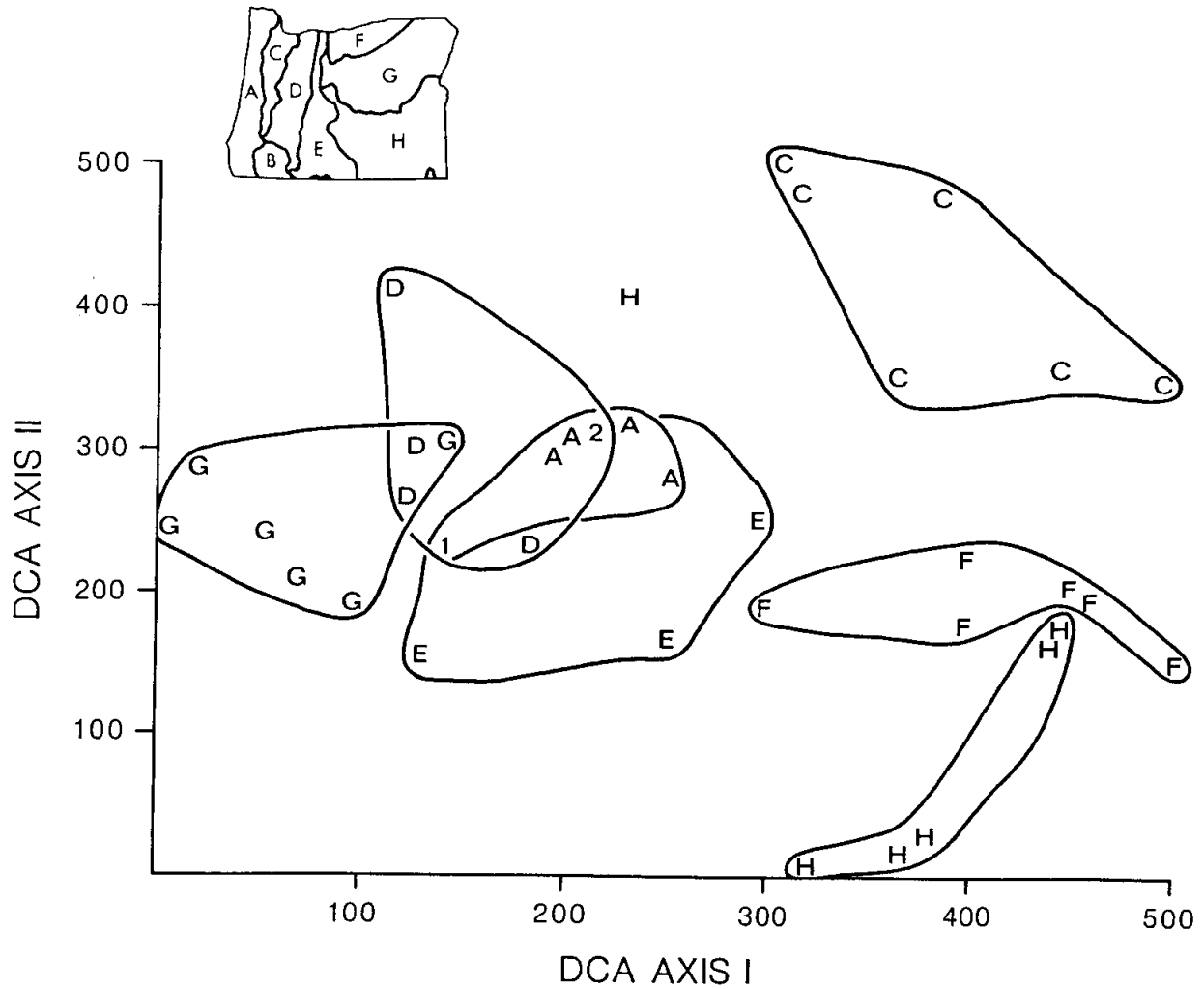
Figure 3.   Regional patterns in Oregon fish assemblages (from Whittier et al. 1988).   A = Coast
Range, B = Sierra Nevada, C = Willamette Valley, D = Cascades, E = Eastern Cascades
Slopes and Foothills, F = Columbia Basin, G = Blue Mountains, H = Snake River
Basin/High Desert. 1 = sites with 100% rainbow trout, 2 = sites with only rainbow trout
and reticulate sculpin.

Table 2. IBI Metrics and Examples of Scoring Criteria

Metric	Scoring Criteria (%)		
	5	3	1
Number of native fish species[a]	>67	33-67	<33
Number of darter/benthic species[a]	▪	▪	▪
Number of sunfish/water column species[a]	▪	▪	▪
Number of sucker/long-lived species[a]	▪	▪	▪
Number of intolerant species[a]	▪	▪	▪
Total number of individuals[a]	▪	▪	▪
Top piscivorous individuals	>5	1-5	<1
Tolerant individuals	<10	10-25	>25
Omnivorous individuals	<20	20-45	>45
Insectivorous individuals	>45	20-45	<20
Exotic or hybrid individuals	<2	2-9	>9
Individuals with disease or anomalies	<1	1-5	>5

(From Karr et al. 1986, Ohio EPA 1988, Miller et al. 1988)

[a]   Determined by maximum species richness (or total abundance) lines (Karr et al. 1986, Ohio EPA 1988) drawn from available data.
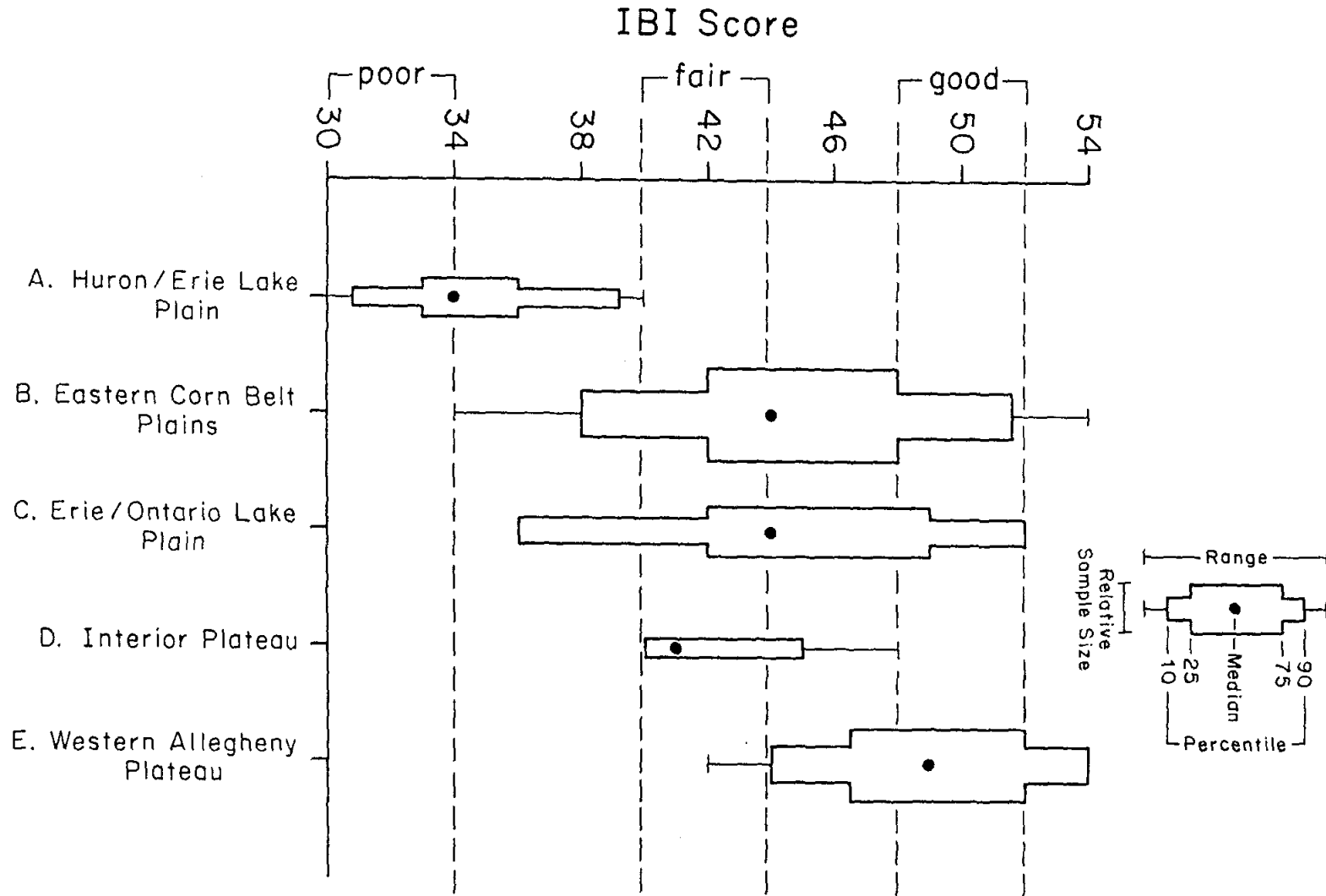
IBI Score

Figure 4.   Index of Biotic Integrity (IBI) values for Ohio ecoregional reference sites (from Whittier et al. 1987). Protective expectations for one region may be underprotective or unreasonable for another.
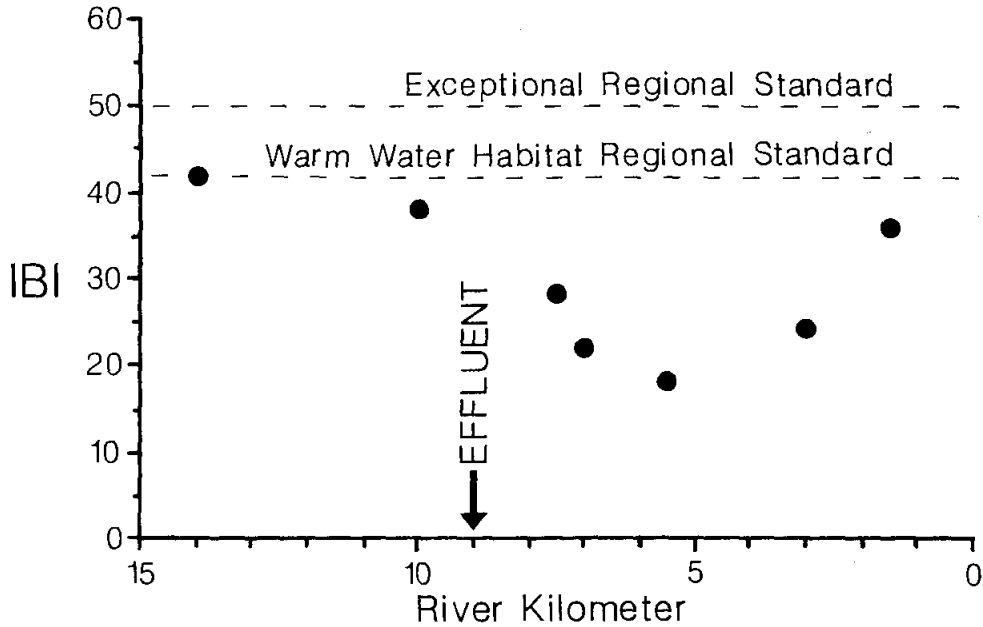
Figure 5. Recovery of Yellow Creek, in Ohio's Erie/Ontario Lake Plain ecoregion (from Ohio EPA 1988). No part of the creek, including the segment above the pollution source, is attaining the regional "exceptional" standard IBI value of 49, which is based on the 75th percentile in Figure 4 and allows for a 4-point IBI uncertainty. One-third of the creek is attaining the regional "warmwater habitat" standard of 42 (25th percentile).
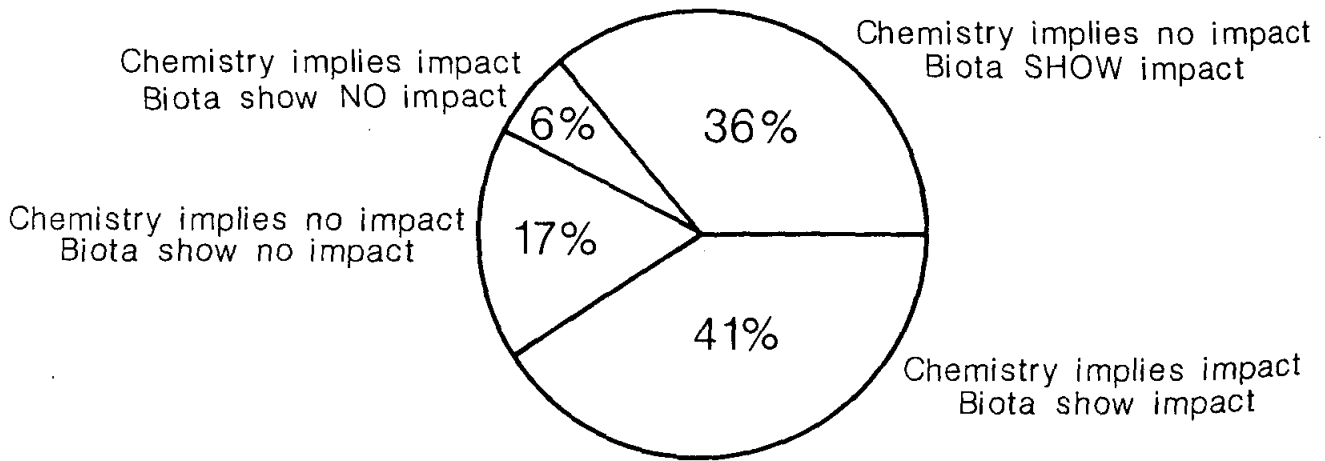
Figure 6. Discrepancies between chemical and biological assessments of impacts evaluated at 431 point source sites in Ohio (Gallant et al. 1989). Biotic impacts, where none are predicted from chemistry, apparently resulted from physical habitat perturbations. This figure suggests that biological evaluations may provide greater protection of Ohio surface waters than do chemical/toxicological assessments.

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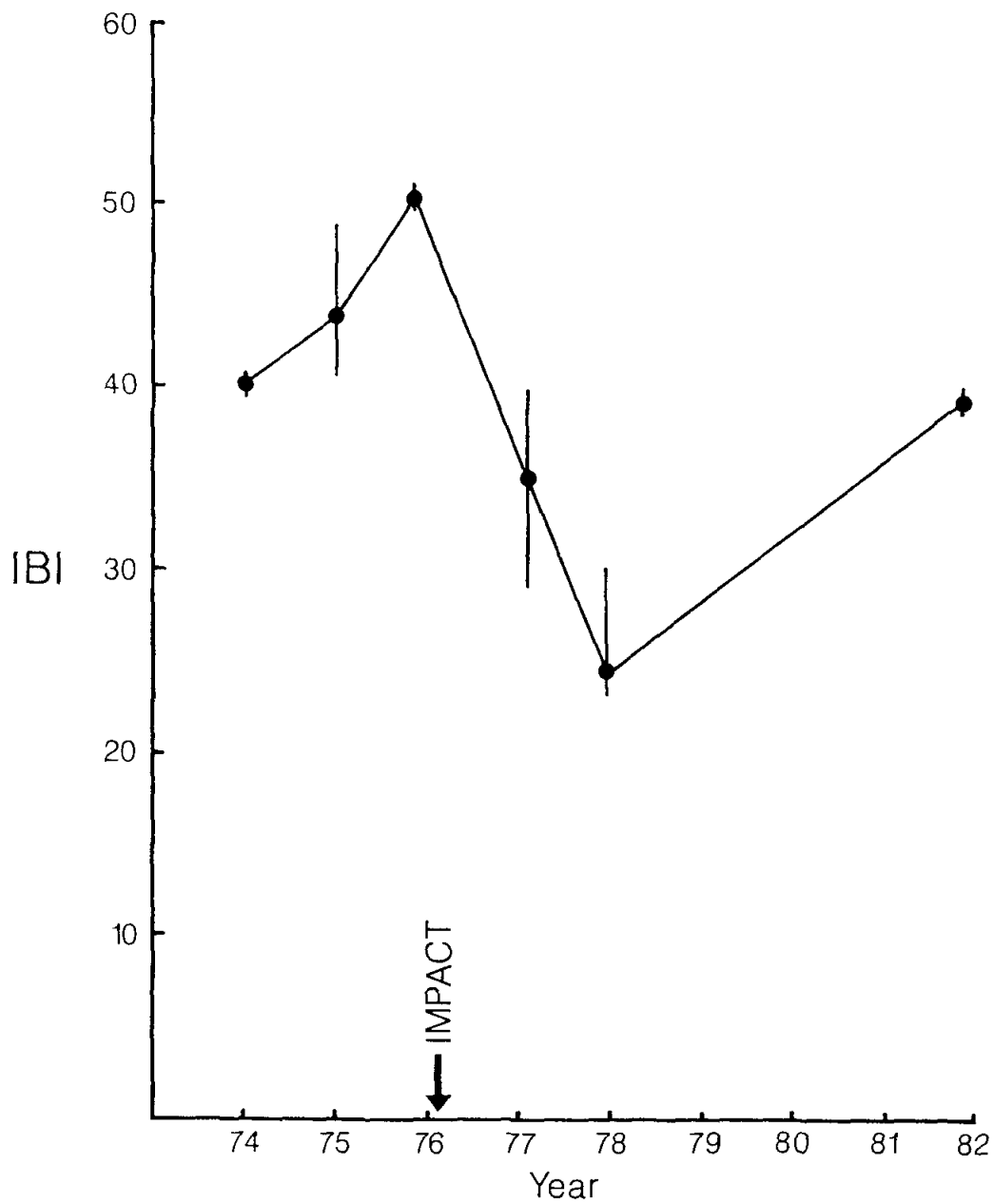
Figure 7.   Temporal trend in Wertz Drain at Wertz Woods, Indiana, stressed by sediment (from Karr et al. 1986).   Vertical lines represent ranges in seasonal samples.   This multiyear sedimentation impact would not have been detected by water quality monitoring.
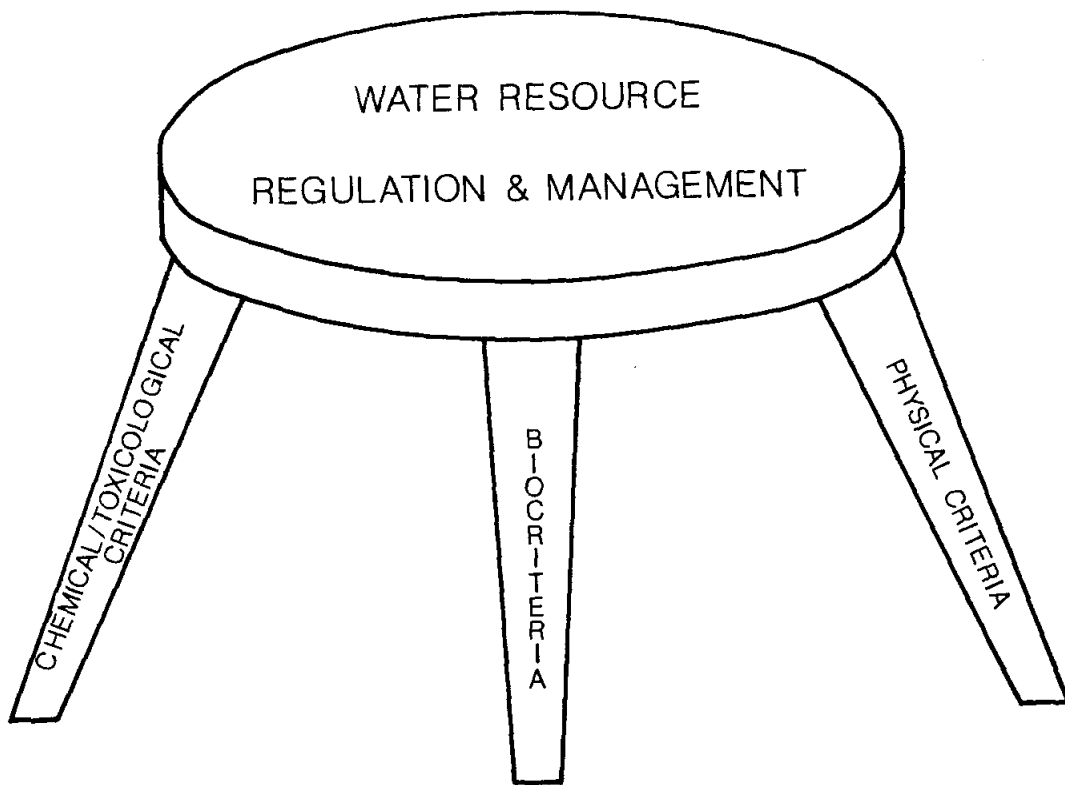
Figure 8.   Just as a three-legged stool is more stable than a one- or two-legged stool, regulatory
criteria and decisions based on biological, physical, and chemical/toxicological monitoring
offer a more stable foundation for water resource management.

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TESTING FOR TREND IN WATER QUALITY DATA

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INTRODUCTION

The Acid Precipitation Act of 1980 (PL 96-294, Title VII) has, as one of its major purposes, the evaluation of environmental effects of acid precipitation. To accomplish this purpose, it is desirable to evaluate the statistical significance of apparent trends in water quality which could be related to acid precipitation. This information goal can be translated into a statistical hypothesis which can be tested using monitoring data. An appropriate null hypothesis would be:

"There are no long-term regional trends in acidification or recovery of surface waters."

The alternate hypothesis is that a trend exists.

A more specific monitoring objective may be stated as follows:

To detect monotonic trends (generally increasing or generally decreasing over time) in data series, both seasonal and annual, for selected water quality variables in individual lakes at the 95 percent (or other stated) confidence level.

This paper discusses the selection of trend analysis methods which are well matched to the statistical characteristics of lake quality data series. The water quality variables of most interest are acid neutralizing capacity (ANC), sulfate concentration, and pH. The primary statistical characteristics of concern are distribution shape (normality versus non-normality), seasonal variation and serial correlation.

In order to select statistical tests which are well matched to both the goals and anticipated data attributes, background data from several sources were studied. Data sources included the "LTM" data set described in Newell (1987), data from Environment Canada for Clearwater Lake, Ontario, and data from the U.S. Bureau of Reclamation for Twin Lakes, Colorado. From these data, generalizations were made regarding the level of seasonal behavior, serial correlation and non-normality to be anticipated.

As a result of this study, data are expected to be seasonal in both mean and standard deviation, to be normally distributed in some cases and non-normally in others, and to occasionally exhibit low level serial correlation for quarterly observations. No conclusions regarding serial correlation of annual values were drawn.

In view of these data characteristics, several candidate tests for trend were selected for evaluation. These tests included both parametric and non-parametric approaches. Several options for dealing with seasonality were included, and one test included a correction for serial correlation.

The candidate tests were evaluated by comparing their performance under a Monte Carlo simulation study designed to reproduce the data characteristics anticipated. The performance indices were actual or empirical significance level and power of trend detection.

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METHODS

As stated earlier, the goal of monitoring which is relevant to this discussion is to determine whether general increases or decreases in observed values of water quality variables are statistically significant--as opposed to being the coincidental result of random or natural variability. The term "trend detection" might therefore be somewhat misleading. It is not generally possible for statistics to detect trends which are not apparent by inspection, especially for data records of short to moderate length--say 20 years or less. Rather one wishes to have a quantitative basis for deciding whether apparent trends are significant.

Statistical tests for trend address the following question: "Given the observed variability in a set of observations, what is the probability that an observed pattern (of increases or decreases) resulted from a no-trend situation?" If this probability is higher than some prespecified level, called the significance level, the null hypothesis of no trend is accepted. If the probability is lower than the significance level, the null hypothesis is rejected.

For clarity let us formally define three terms as follows:

1. Trend is a general increase or decrease in the value of observations of a particular variable over time. For the purpose of comparing statistical tests, trends are later assumed to be monotonic (one directional) and gradual (linear) for simulation purposes.

2. The "significance level" of a test, denoted by α, is the probability of rejecting the null hypothesis of no trend when it is true. The significance level is also referred to as the type I error. The "nominal significance level" of a test is the rejection probability when all of the assumptions underlying the test are satisfied and the test statistic follows its theoretical distribution. The nominal significance level is usually specified before a test is run. In practice, the assumptions associated with a given test are not

satisfied exactly, and the true or "actual significance level" will be different from the nominal level. In water quality monitoring, the assumptions underlying tests may be seriously violated, and the actual significance level may be quite different from the nominal level. Since one's knowledge of the variables being monitored is quite limited, however, the actual significance level is never known. One can only minimize the difference between nominal and actual levels through the use of tests which are either based on assumptions which closely match the data characteristics and/or which are insensitive ("robust") to violations of underlying assumptions.

3. The "power" of a test is defined as the probability of rejecting the null hypothesis when a trend really exists. Power may also be defined as $1-\beta$ where β is the Type II error or probability of accepting the null hypothesis when it is false (when a trend really exists).

One would like to maximize the power of a test and minimize the significance level. Unfortunately there is a direct relationship between the two. For given population characteristics and given sample size, the power of a given test decreases with decreasing significance level. Thus one is forced to make do with some sort of trade-off between the two (at least in the usual situation where both the resources and direction of a monitoring program limit the effective independent sample size available for testing).

The power of a test also depends on the nature of the trend which really occurs. By "nature" of trend one means the functional form (gradual, sudden, linear, polynomial, monotonic sinusoidal, etc.); the magnitude and duration; and the population changes such as changing variance, which accompany or are considered part of the trend.

In the real world, the possibilities (for nature of trend) are literally endless. One therefore has no way to specify the power of a given test a priori. However, using

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hypothetical trend models, one can identify the power of a given test under those trend models and use the results to objectively compare the performance of alternative statistical tests. Similarly one can use models of no-trend conditions to compare the empirical (actual) significance levels of candidate statistical tests. This approach, limited simulation of water quality random variables under assumed behavioral characteristics, was used here to compare alternative trend tests.

Seven statistical tests for trend were selected as candidates for evaluation. The selection was based on the results of background data characterization and on a review of the statistical and hydrological literature. The candidate procedures were as follows:

1. Analysis of covariance (ANOCOV) on raw data

2. Modified "t" on raw data

3. Kendall tau on deseasonalized data (also called the Kendall Rank Correlation test or Mann-Kendall test for trend)

4. Seasonal Kendall with correction for serial correlation

5. Seasonal Kendall

6. Analysis of covariance (ANOCOV) on ranks of data

7. Modified "t" on ranks of data

A brief discussion of these procedures follows.

Analysis of covariance (ANOCOV) is based on a linear model and normal theory (Neter and Wasserman, 1974). The trend test is simply multiple linear regression of a water quality (dependent) variable against two or more predictive (independent variables). One of the dependent variables is time, and the rest are seasonal indicator variables. For quarterly observations, three indicator variables are used, corresponding to any three of the four seasons--for example, winter,

spring, and summer. To indicate a winter observation, the first indicator variable would be set equal to one and the rest equal to zero. For spring observations, the second indicator variable would equal one, the rest zero. If all three indicator variables are zero, a fall observation is indicated.

The regression calculates three seasonal or coefficent terms and an overall intercept. The slope against time is tested for significance using a null hypothesis that the slope is zero. If the null hypothesis is rejected, one concludes that there is a significant (linear) trend in the data.

The ANOCOV procedure assumes homogeneous (constant) variance across all seasons. Since we expect TIME data to exhibit seasonal changes in variance, however, another test was developed which does not assume homogenous variance. The test, called the modified "t", involves a separate linear regression of the water quality variable against time in each season. The regressions are followed by a test of the null hypothesis that the sum of the regression slopes (four slopes for quarterly data) is equal to zero. If all slopes are assumed to be in the same direction, this condition is satisfied only if there is not overall (linear) trend. If the null hypothesis is rejected, one concludes that there is a significant overall linear trend.

The Kendall-tau procedure is described in Snedecor and Cochran (1980). The method is non-parametric, meaning that it does not depend on an assumption of a particular underlying distribution. The procedure tests for correlation between the ranks of data and time and as noted by Gilbert (1987) "can be viewed as a non-parametric test for zero slope of the linear regression of time-ordered data versus time, as illustrated by Hollander and Wolfe (1973, p.201)." Since the test depends only on relative magnitudes of data rather than actual values, it may also be viewed as a test for general monotonic trends rather than specifically linear trends.

Seasonal variation should be removed from a data series prior to the application of this test. This is accomplished by computing seasonal means (for example, the sample

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mean of all fall values) and subtracting the appropriate season mean from each observation. The procedure utilized herein is to subtract seasonal means without any prior test for seasonality. In other words, all data series are assumed to be seasonal and are "deseasonalized" prior to applying Kendall-tau. Of course for annual data in which all observations are from the same time of year, the deseasonalizing" step is not necessary.

The Seasonal Kendall test as described in Hirsch et al. (1982) is an extension of the Kendall-tau test. The Seasonal Kendall test statistic is the sum of Kendall-tau statistics computed for each season (month or quarter, for example) of the year. This test accounts for seasonal variation directly and does not require prior removal of seasonal means.

The sixth and seventh procedures are identical to the first and second with one exception. The data are first ranked, and the ranks are substituted for the original values of the observations. The rank transformation is suggested by Conover (1980).

The fourth and fifth procedures are identical with one exception. In the fourth prcedure the variance of the Seasonal Kendall test statistic is corrected by including a covariance term which reflects serial correlation of observations. The modification is described in Hirsh and Slack (1984).

Two key assumptions of the various tests should be emphasized at this point. First is the form of trend assumed. The analysis of covariance model assumes a linear trend component, the modified "t" assumes a linear trend within each season. Although the tests are certainly appropriate for more general trends (gradually increasing or decreasing but not necessarily in a straight line), one should keep in mind that our comparisons were based on linear trend. Thus they slightly favored these two tests.

The ANOCOV and modified "t" on ranks make the same assumptions, but on the ranks of data rather than the actual observations. Thus linear trends in the observations are not assumed, but one does assume that the form of the trend is gradually increasing or

decreasing. The Kendall tau and Seasonal Kendall test are designed for general monotonic trend. Thus they would be regarded as more general than the other tests.

In fact any of the tests could be applied to a wide variety of trend shapes, including quadratic or step trends. If trends are not monotonic, meaning that the general tendency would be in one direction for a while and then reverse, the tests would not be very sensitive unless there were a clear overall tendency either up or down. Thus one would generally want to inspect time series plots before performing the tests in order to identify segments which have differing trend directions or other characteristics which indicate that more in-depth treatment is necessary.

The second key assumption is independence of observations. All of the tests account for seasonal dependence in some way or other; however, only the corrected Seasonal Kendall test accounts for serial correlation—temporal dependence after seasonality is removed. All of the other tests assume that samples are independent in the absence of seasonality (i.e. there is no serial correlation).

While we do not believe that quarterly observations will exhibit strong levels of serial correlation, one should realize that any serial correlation will affect the performance of the tests. Specifically the tests will tend to reject the null hypothesis more often than they should. The correlated series will tend to "drift" above or below the long-term mean and stay there for a while, and this "drift" will sometimes be indistinguishable from trend depending on the time horizon over which the process is viewed. (The term "drift" has a particular connotation in stochastic modeling which is not intended here.)

In practice, the classification of observed patterns as either trend or serial correlation is rather subjective. There is no way to overcome this difficulty without very long records or physical explanations for observed patterns. Thus we have not spent a great deal of time in working on methods to account for serial correlation in trend analysis.

MONTE CARLO EVALUATION OF CANDIDATE TESTS

Since analytical evaluations of power and significance levels are possible only in a limited number of situations, a good comparison of trend testing methods, is best achieved through Monte Carlo testing. In a Monte Carlo evaluation, the significance level of a test is determined by generating a large number (say 500) of sequences of data with known characteristics and no trend. The test is applied to each sequence, and the significance level is the fraction of trials in which a trend is falsely detected.

The power of a given test is determined in the same way except that a trend of known magnitude is added to each synthetic data sequence. The power is the fraction of sequences in which the trend is correctly detected.

To compare alternative tests we need to perform a very large number of simulation experiments. Time series of several types must be considered. To adequately represent the range of characteristics anticipated, the parameters which should be varied are magnitude of seasonality in mean, pattern of seasonality in mean, magnitude and pattern of seasonality in variance, normal versus non-normal distribution, degree of serial correlation, trend magnitude, and length of record. The number of possible combinations of these parameters is very large, and rigorous testing of all possibilities would require an enormous amount of computer time.

Therefore, we developed a limited Monte Carlo testing program which looked at a few key values of the above parameters based on our historical data analysis and tried all possible combinations thereof. The simulations are described in Table 1. Only normal and log normal distributions were considered; and only simple AR(1) type autocorrelation was considered. Autocorrelation was not considered for the log normal case. Even with these simplifications, 3456 combinations of parameters were evaluated. For each combination, at least 500 sequences were generated to empirically determine the power

or significance level of the candidate tests. All candidate tests were applied to each synthetic data sequence.

RESULTS

The most powerful tests over the range of conditions studied appear to be the Seasonal Kendall test and ANOCOV on ranks, although as expected, no single test performs best under all conditions. Both of these tests performed as well as the parametric tests when the data were normal and both out performed (were more powerful than) the parametric tests when the underlying distribution was log normal. In a few cases, the Kendall-tau on deseasonalized data was more powerful, but it did not generally preserve the nominal significance level as well as the other tests. The modified "t" test on ranks performed well, but was in most cases slightly less powerful than ANOCOV on ranks.

All tests except the corrected Seasonal Kendall (#4) suffered from inflated significance levels under serial correlation. The corrected test, however, is much less powerful than the other tests except for very large trend magnitudes and/or long data records. As expected, it is very difficult to distinguish between linear trend and serial correlation.

This test is not recommended for routine application until very long records (say > 20 years of quarterly data) have been obtained. The correction for serial correlation will cause the test to "ignore" trends of moderate magnitude and duration which may be important from a management standpoint. The question of whether a change in water quality is of interest is one of physical causality. Persistence in the series, as described by a correlated process model, would be caused by some factors which are not of interest (say long lake retention time) and others which are of interest (say cycles of industrial activity). We would argue that it is wise to "detect" more trends, some of which are "false positives" and to then screen according to probable cause than to overlook more changes which are really of interest.

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TABLE 1. Description of simulations for Monte Carlo testing
program.

A. Seasonal patterns in mean

    Pattern (1)   Quarter 1 - Low
                   Quarter 2 - High
                   Quarter 3 - Low
                   Quarter 4 - Low

    Pattern (2)   Quarter 1 - Low
                   Quarter 2 - High
                   Quarter 3 - Low
                   Quarter 4 - High

B. Seasonal patterns in standard deviation
      (same two patterns as in mean)

C. Ratios of largest to smallest quarterly standard
   deviation

      1.0, 1.5, 3.0, 5.0

D. Ratio of largest to smallest quarterly mean

      1.0, 1.5, 2.0

E. Trend magnitude = $\dfrac{\text{(change in mean per sampling interval)}}{\text{(average standard deviation over all quarters)}}$

      0.0, 0.002, 0.005, 0.02, 0.05, 0.2, 0.5

F. Length of record (years)

      5, 15, 25

G. Underlying distribution

      Normal, log normal

H. Lag-one autocorrelation coefficient $\rho(1)$ =

      0.2, 0.4
      (Correlated sequences generated for normal data only.)

I. Nominal significance level α = 0.05 for all tests.

In fact, we believe that it will probably not be possible to deal satisfactorily with the issue of serial correlation with any routine time series approach until very long records are available. Although several methods are available, such as ARIMA modeling of the time series and extension of linear regression, all require some type of estimation of the correlation structure of the series of interest. The trend test is then modified in some way to account for the correlation. However, there is no way to uniquely characterize a correlated time series with small sample sizes. Only for large sample sizes, therefore would more complex time series methods be justified.

CONCLUSIONS AND RECOMMENDATIONS

As stated earlier, the two recommended tests out of the seven candidates are ANOCOV on ranks and Seasonal Kendall.

ANOCOV on ranks offers the advantage of being insensitive to the pattern and magnitude of seasonal change in variance. It is also easily applied by anyone who has a microcomputer stat package with the capability of multiple linear regression. ANOCOV is also a very flexible method. The general ANOCOV model and procedure can be expanded by adding covariates to achieve additional power or increased ability to explain trends.

On the other hand, the Seasonal Kendall test has a proven "track record" in water quality data analysis (Smith et al., 1987) and offers slightly better performance under certain conditions, notably the presence of serial correlation. For these reasons, the authors have a slight preference for the Seasonal Kendall test. We recommend including ANOCOV on ranks as an alternative because of its ease of application with "stat packs" and its potential for extension to multivariate tests.

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