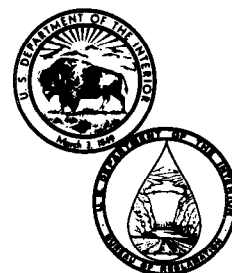REC-ERC-83-12

MICROSYSTEM SEDIMENT-WATER SIMULATION: A PRACTICAL TECHNIQUE FOR PREDICTING RESERVOIR WATER QUALITY

October 1983
Engineering and Research Center

U. S. Department of the Interior

Bureau of Reclamation

TECHNICAL REPORT STANDARD TITLE PAGE

1. REPORT NO. **REC-ERC-83-12**	2. GOVERNMENT ACCESSION NO.	3. RECIPIENT'S CATALOG NO.
4. TITLE AND SUBTITLE **Microsystem Sediment-Water Simulation:** **A Practical Technique for Predicting** **Reservoir Water Quality**		5. REPORT DATE October 1983
		6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S) **Douglas Craft**		8. PERFORMING ORGANIZATION REPORT NO. REC-ERC-83-12
9. PERFORMING ORGANIZATION NAME AND ADDRESS Bureau of Reclamation Engineering and Research Center Denver, Colorado		10. WORK UNIT NO.
		11. CONTRACT OR GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS Same		13. TYPE OF REPORT AND PERIOD COVERED
		14. SPONSORING AGENCY CODE DIBR

15. SUPPLEMENTARY NOTES

Microfiche and/or hard copy available at the E&R Center, Denver, Colorado

Ed: RNW

16. ABSTRACT

Water quality at the bottom of a lake or reservoir may be conveniently simulated in a controlled laboratory environment using the technique of microsystem sediment-water simulation. The technique provides predictive data on planned or existing reservoirs and lakes by duplicating conditions expected at the sediment-water interface including anaerobic (chemically reducing) conditions which may occur in the hypolimnion during summer and winter stratification. Using many small sediment-water "microsystems" allows for replication and the estimation of experimental error, as well as application of a variety of analytical chemical techniques for characterizing the simulation water. Also, the relatively small size of microsystems offers economies of scale advantages compared to some previously suggested simulation techniques. A general methodology is presented along with a discussion of microsystem advantages and disadvantages.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS-- soil samplers/ water sampling/ *water quality/ water analysis/ water chemistry/ *ecosystems/ hypolimnion/ stratification/ *reservoir surveys

b. IDENTIFIERS--

c. COSATI Field/Group 08 14   COWRR: 14 02   08 08   SRIM:

18. DISTRIBUTION STATEMENT (Microfiche and/or hard copy available from NTIS)	19. SECURITY CLASS (THIS REPORT) UNCLASSIFIED	21. NO. OF PAGES 7
	20. SECURITY CLASS (THIS PAGE) UNCLASSIFIED	22. PRICE

REC-ERC-83-12

MICROSYSTEM SEDIMENT-WATER SIMULATION:
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October 1983

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Division of Research
Engineering and Research Center
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ACKNOWLEDGMENTS

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APPLICATION

The methodology presented in this report would be of interest to design engineers and planners involved in environmental impact analysis for proposed reservoirs, as well as operation and maintenance personnel who are concerned with water quality problems in existing reservoirs. This report also would interest environmental scientists involved in research on nutrient and trace metal cycling in lakes and reservoirs, and researchers concerned with the effects of acid precipitation on aquatic ecosystems.

SUMMARY AND CONCLUSIONS

1. Reservoir simulation is a predictive water quality technique which provides data more closely related to expected natural conditions than are available from techniques currently used during environmental impact analysis for proposed reservoirs.

2. The procedures outlined in this report have been tested and evaluated on a proposed reservoir site in Utah; data from this study are available in another report [1].*

3. Microsystem simulation is a straightforward technique applying existing technology and methods. The necessary equipment is available commercially at reasonable cost.

4. Sample preparation methods suggested for anaerobic microsystems result in minimal changes in the water chemistry prior to chemical analyses.

5. Using microsystems allows for replication in chemical analyses and, thus, a more accurate estimate of experimental error is obtained.

6. Because all of the microsystem water is prepared for chemical analyses, the problem of microstratification — noted in larger sediment-water systems — is reduced. Microsystems are easier to seal, which minimizes the chance of oxygen contamination.

7. Since microsystems represent a static simulation, data obtained using this technique represent "worst case" rather than "actual" water quality conditions.

8. The validity of microsystem simulation predictions will depend ultimately on whether postimpoundment limnological survey results corroborate simulation data.

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* Numbers in brackets refer to the bibliography.

INTRODUCTION

Chemical analysis surveys of streams and soil are commonly performed as part of the environmental impact analysis for a proposed reservoir. These data are used to estimate the expected reservoir water quality either by comparison to existing reservoirs or with the aid of computer models. While providing valuable information, the accuracy of predictions based on chemical analyses surveys is limited by the inherent complexity of reservoir ecosystems and the lack of selectivity in chemical analysis methods.

Stream water-quality data are limited as a basis for predictions of reservoir chemistry because reservoirs – like lakes – exhibit thermal stratification during summer and winter. One major consequence of thermal stratification is the development of anaerobic (without oxygen), chemically reducing conditions in the reservoir hypolimnion. This may lead to the release of nutrients and toxic metals from hypolimnetic sediments. Additionally, the variety of land use patterns surrounding a reservoir, differing soil types, and influent and effluent flow regimes will result in microenvironments within a reservoir with water quality different from the rest of the reservoir.

Predictions based on chemical extractions of soil samples usually provide data with little relation to the real reservoir conditions. For example, trace metals usually are extracted from soil using high-temperature digestions with strong acids and oxidizing agents. Such extreme treatment yields total metal concentrations having little information regarding the availability or solubility of trace metals once the reservoir is filled. Selective extractions which use various buffer solutions and/or complexing agents as the extractants may be used to estimate long-term releases of nutrients and metals from aerobic sediments [2]. However, these techniques cannot predict the response of a natural system to changing influent water quality, land use patterns, or the nutrient and metal releases expected from anaerobic sediments.

In addressing the problem of reservoir complexity, researchers at the Waterways Experiment Station, U.S. Corps of Engineers, Vicksburg, Mississippi, developed a predictive water-quality technique that simulates the reservoir sediment-water interface [3]. The technique involves sealing sediment and water from a proposed reservoir in large (about 250 L) Plexiglass vessels, which are then incubated in a controlled light and temperature room. As the sealed sediment-water systems develop anaerobic conditions, the water is sampled for chemical analyses. Therefore, with certain limitations, simulation in a controlled laboratory environment is able to mimic

the processes expected to occur in the reservoir hypolimnion.

Reservoir simulation offers several advantages over other predictive water-quality methods. The principal advantage is that data are obtained from direct measurements on a quasi-natural system, providing a more accurate representation of possible future conditions. Another advantage is the ability to simulate many locations within a proposed reservoir, allowing the identification of problem areas and providing data related to the range of possible water-quality conditions to be expected. Additionally, the technique may be applied at existing lakes and reservoirs to resolve questions related to nutrient and trace metal cycling, or to ascertain the response of a natural system to chemical perturbations, such as increased nutrient inflows or acid precipitation effects.

The simulation methodology in this report represents modifications of methods suggested by Gunnison, et. al. [3, 4], and differs from other methods in that the large sediment-water system is replaced by many smaller "microsystems." The use of microsystems offers several advantages over previously suggested methods and should enable wider use of reservoir simulation as a water-quality evaluation tool.

METHODOLOGY

The methods suggested here represent general guidelines for those who plan microsystem simulation studies. There are no rigid rules, since each reservoir represents a unique system complete with its own set of distinctive features and problems.

Site Selection

Some of the reasoning leading to the selection of sampling sites may be outlined by reference to the map on figure 1. Figure 1 represents a hypothetical reservoir in the western United States. The reservoir has a river with two tributary creeks as its major water source. The river exhibits good water quality with relatively low total ion concentrations, and good bicarbonate buffering. Creek A drains an abandoned mining area, is high in sulfate and trace metal concentrations and has a pH of 4.9. Biological activity does not exist in creek A, and the water is colored ocher. Creek B water quality is similar to the river with the exception of high nitrogen and phosphorus concentrations because of agricultural runoff and untreated municipal waste effluent from the farm town. Reservoir basin soils are similar in geologic origin, having high organic carbon concentrations that are observed in soils adjacent to the river.
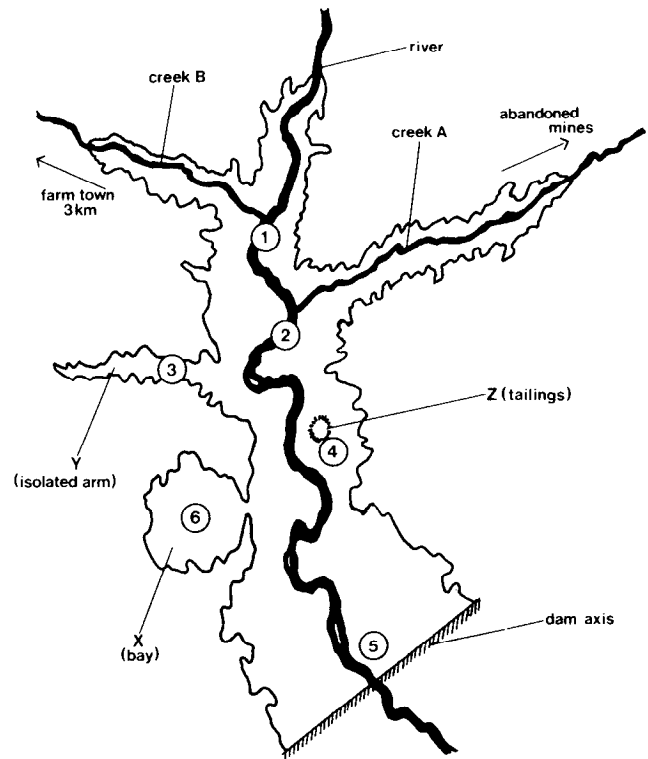

Figure 1.–Map of a hypothetical reservoir.

Physical features of this hypothetical reservoir include arms associated with each inflow, an isolated bay (labeled X), and another arm which lacks an inflow except for storm runoff (labeled Y). There is an abandoned mine-tailings pond in the middle of the proposed reservoir basin (labeled Z) that is high in metal concentrations and acidity. The reservoir is expected to have an average depth of 90 meters at the deepest point (near the dam). Computer temperature models predict a thermally stratified system.

Note that six proposed sampling sites (numbered 1 to 6) are indicated on the map. Sites 1 and 2 are located just below the confluences of the creeks and the river. Site 5 is located in rich river-bottom soils at the deepest part of the reservoir. The remaining sites represent areas where water quality problems are expected. Sites 3 and 6, which lack inflows and are relatively isolated from the main reservoir body, probably will experience stagnation and prolonged anaerobic conditions during episodes of thermal stratification. Site 4, in the acidic mine-tailings pond, is an obvious choice due to the high concentrations of metals expected to be released. Site 2 is important because of poor water quality associated with drainage from the abandoned mining area along creek A.

Generally, any site which may present a water-quality problem, either as a pollution source or location of

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poor mixing should be considered for simulation. It is equally important to select sites that will provide data related to "average" or overall reservoir conditions; site 5 (near the dam) is an example of such a location. Choosing problem-free sites also provides some idea as to the range of possible water-quality conditions to be expected in the reservoir.

It should be noted that any decision on site selection must depend on a reasonable amount of preliminary survey data at the reservoir site and a careful evaluation of the anticipated reservoir operation and use patterns.

Equipment

The following is a list of equipment and material required:

> 19-L (5-gal) plastic buckets with sealable lids

2. 19-L (5-gal) plastic "jerry" cans
3. 500-mL, wide-mouth Erlenmeyer flasks
4. No. 10 neoprene stoppers
5. 4.75-mm sieve (U.S.A. Standard sieve No. 4) and standard soil preparation equipment
6. Temperature-controlled incubator, 0 to 25 °C (0 to 77 °F)
7. Controlled-atmosphere glove box
8. Vacuum pump
9. Argon (welding grade) tanks with regulators
10. Membrane filtration apparatus (glass) with 0.45-μm membrane filters
11. pH-millivolt meter with combination pH electrode and combination platinum redox electrode
12. Magnetic stirrer with Teflon-coated stirring bars
13. Deionized water source

Soil Sampling

After simulation sites have been chosen, the following procedure may be used to obtain the necessary soil samples:

1. Before leaving for the site, one sealable, 19-L plastic bucket per sampling site, as shown on figure 2, should be washed thoroughly and then rinsed with 10 percent (volume percent) HCl (hydrochloric acid). After the HCl rinse, the bucket should be rinsed five times with deionized water.

2. Upon arrival at the sampling location, use a shovel to obtain surface soil (the upper 30 mm) from about a 100-m² area. For best results, take the surface soil in random shovelfuls within the sampling area to obtain a good composite sample of about 10 kg.

3. Document the location adequately and note the vegetative cover and soil color and texture. Photographs are a valuable supplement to documentation. Label the bucket containing the composite soil sample and then seal the bucket lid, using heavy-duty duct tape. The sample is now ready for shipment.

Existing reservoirs and lakes may be simulated by collecting bottom sediments, rather than preimpoundment soil. Sediments should be collected by using a bottom dredge, drained of excess water, sealed in a suitable container, and refrigerated during shipment.

Water Sampling

Water sampling locations should be somewhat downstream of the particular soil sampling site (about 100 m) to ensure that the water quality corresponds to the influent conditions expected in the reservoir at the sampling site. For example, in the hypothetical reservoir, site 1 water should not be used for site 6 sediment-water microsystems, since site 1 water would not contain the effluent from the abandoned mining area. Water may be collected conveniently in 19-L plastic "jerry" cans which previously have been rinsed with 10 percent (volume percent) HCl and then rinsed five times with deionized water. The "jerry" cans should be rinsed three times with river or stream water before filling. After being filled, the water should be kept cool and in the dark until ready to be introduced into the microsystems.

Microsystem Preparation

Soil samples are air dried and then passed through a 4.75-mm sieve (U.S.A. Standard sieve No. 4). Large soil clods are broken with a wooden mallet. Rock, sticks, and other objects larger than 4.75 mm are removed. The material passing the sieve then is blended and split into representative quarters for

Figure 2.–Plastic buckets used to collect soil samples for simulation studies. P801-D-80333

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ease of handling during subsequent splitting for preliminary chemical analyses and microsystem preparation. Care should be taken to ensure that proper soil preparation procedures are followed. Sediment samples from existing reservoirs should be dried and prepared using these suggested procedures for soil preparation.

Microsystem simulation is performed using 500-mL, wide-mouth Erlenmeyer flasks which previously have been washed in 10 percent (volume percent) HCl and rinsed five times with deionized water. A 40.0-gram $\pm$ 0.1-g, air-dried representative soil or sediments sample is placed in each flask with 500 mL of water appropriate to the site. Figure 3 shows an example of microsystems. A typical simulation study requires about 36 microsystems for each selected site.

Before degassing and sealing, each microsystem should be shaken several times and allowed to settle overnight while in atmospheric contact. This procedure allows the removal of floating organic material, and simulates the mixing expected when the soils are initially flooded.

It has been observed that degassing of microsystems is sometimes necessary to promote the development of anaerobic conditions within a reasonable time (1 to 3 weeks). Microsystems may be degassed in the vacuum/transfer chamber part of a glove box by applying a vacuum for 30 minutes with periodic vibrations to dislodge gas bubbles as shown on figure 4. This treatment will reduce D.O. (dissolved oxygen) concentrations in the microsystems to below 0.1 mg/L. Once degassed, the microsystems are ready to be transferred to the glove box interior for sealing. Prior to transferring the degassed microsystems to the glove box interior, the glove box should be evacuated to a slight negative pressure and then filled with argon gas to a slight positive pressure four complete times. Sealing and subsequent sample preparation should be performed under a slightly negative inert atmosphere to facilitate the use of gloves and to inhibit diffusion of gas into the microsystem water. Microsystems sealed with No. 10 neoprene stoppers may be secured with fiber packing tape wrapped around the vessel and stopper.

The sealed microsystems are now ready to be placed in the refrigerated incubator for simulation as shown on figure 5. It is recommended that the microsystems be incubated at a temperature consistent with a reservoir hypolimnion of similar depth, altitude, and latitude, and that simulations be performed in the dark.
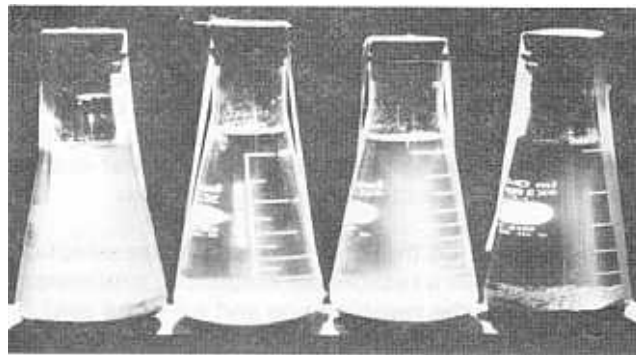

Figure 3.–Sediment-water microsystems. P801-D-80334

Figure 4.–Controlled-atmosphere glove box used for anaerobic sample preparation. P801-D-80335

Simulation Sample Preparation

At selected intervals, microsystems are removed from the refrigerated incubator for sample preparation before chemical analyses. Several prepared microsystems should be analyzed prior to being degassed to provide baseline data for aerobic reservoir conditions. Gross water-quality parameters such as pH and Eh (redox potential) should be measured and samples for nutrients and trace metals are usually filtered through a 0.45-μm membrane filter. The

Figure 5.–Controlled-temperature incubator. P801-D-80336

principal requirement is that any sample preparation be performed in the glove box under a slightly negative inert atmosphere once the microsystems have been degassed.

The glove box may be prepared using the procedure suggested for the initial sealing of the microsystems. During a recent simulation study [1], it was observed that sample preparation resulted in minimal changes (3 to 8 percent increase) in the redox potential of the anaerobic microsystems. If the magnitude of such changes is unacceptable, then residual oxygen concentrations in the glove box may be reduced by using an oxygen-absorbing scrubber for the argon and increasing the number of times the glove box atmosphere is exchanged. The important point is to minimize sample preparation effects on the redox condition of anaerobic microsystems.

Figure 6 outlines the sample preparation procedure used during a simulation study for a proposed reservoir in Utah [1]. Note that pH and Eh are measured on each microsystem prior to being combined into a composite sample, and that a replicate composite sample from the same site also is processed for analysis. These procedures allow an estimate of the between-system error and check on the possibility of oxygen contamination.

Another important point concerning figure 6 is the inclusion of a technique for determining the *lability*, or kinetic tendency to dissociate, of trace metal complexes using Chelex 100 chelating ion-exchange resin (Bio-Rad Laboratories). This technique, suggested by Batley and Florence [5], and Figura and McDuffie [6], is a good example of how newer methods which provide more detailed data on simulation water chemistry may be included in simulation studies.

Regardless of the analyses chosen for a simulation study, it is emphasized that all appropriate precautions concerning adequate cleaning of glassware and minimizing of contamination are strictly followed. Also, it is important to include quality control as a part of any analytical work performed.

Proper preservation techniques for samples that cannot be analyzed immediately should be considered. Trace metals are preserved easily by adding ultrapure nitric acid (0.1 percent of total sample volume) after filtration or other preparative technique. Nitrogen and phosphorus samples cannot be preserved with acid, so it is recommended that samples – for each individual analysis – be placed in small sample bottles that are then sealed in "ziplock-type" plastic bags while still inside the inert glove
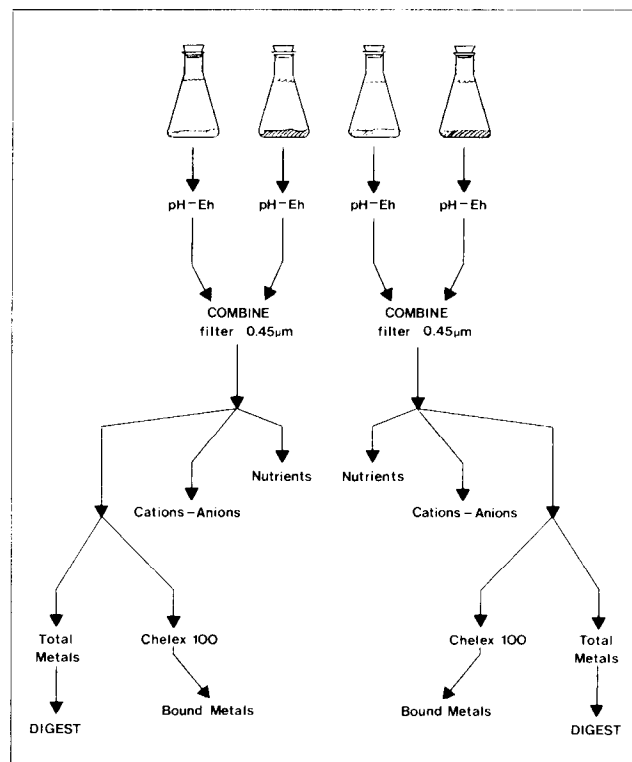

Figure 6.–Chemical analysis flowchart. Chart details microsystem sample treatment procedures followed during a simulation study for a proposed reservoir in Utah.

box atmosphere. These sealed samples may be frozen for preservation until they are ready to be analyzed. Seals on the samples should not be broken until immediately prior to introduction into an instrument or reaction with a colored complex reagent so that minimal changes in sample redox potential, from exposure to atmospheric oxygen, will occur.

DISCUSSION

Microsystem simulation offers several advantages over previously suggested methods which become apparent when anaerobic conditions are present in the sediment-water systems. Anaerobic bacteria are extremely sensitive to oxygen contamination; therefore, leaks are a serious problem in simulation studies. Larger systems are inherently more difficult to seal and require recirculation pumps to overcome chemical microstratification [4]. Recirculating pumps and external sampling devices increase the risk of leaks. Microsystems are small and easier to seal and all the system water is used for chemical analyses. Thus, the problem of microstratification is reduced, because stratified layers of water are included in the composite sample. Additionally, since microsystems are small, they may be transferred (airtight seals intact) to an inert atmosphere glove box for sample preparation. Consequently, the risk of atmospheric contamination is reduced greatly using microsystem techniques.

Another advantage of microsystem simulation is the ability to obtain error statistics by analyzing replicate systems at each sampling. Knowledge of experimental error allows a more reasoned and analytical interpretation of simulation data, especially considering the heterogeneous nature of soils.

Finally, because microsystems are about 400 times smaller than "large" systems, costs associated with the technique reflect the economy of scale. Instead of custom-fabricated sediment-water chambers, 500-mL glass Erlenmeyer flasks may be used. Instead of a temperature-controlled room, microsystems may be kept in a refrigerated incubator (refrigerator) conveniently located in a chemistry laboratory. Savings associated with the microsystem technique should, therefore, appeal to cost-conscious researchers.

While sediment-water simulation represents an improvement over currently used techniques, it is important to note that there are problems with the technique which deserve attention. Previously suggested simulation methods and microsystem simulation use static systems that are unable to simulate the hypolimnetic inflow-outflow conditions usually observed in a reservoir. Thus, static techniques will provide "worst case" data (e.g., when a reservoir experiences prolonged stagnation), rather than "actual" data. Gunnison [3] proposed a flow-through simulation technique which simulates the natural reservoir water exchange; however, size and cost of such a system may be prohibitive to researchers with limited budgets. Microsystem simulation could be adapted for flow-through studies; however, it is not known whether the increased costs and complexity would result in cost-effective improvements in the accuracy of the technique.

Another problem associated with microsystems is the adsorption of chemical species – notably trace metals – on the interior glass surfaces of the flasks. For metals present in the low-microgram-per-liter concentrations, adsorption onto the glass surface may be a serious situation, especially during aerobic conditions. It is recommended that researchers using microsystem simulation techniques be aware of this problem and make an attempt to quantitate adsorption effects.

Finally, it is important to note that the final judgment on the accuracy of microsystem simulation predictions must await postimpoundment limnological verification studies. Microsystem simulation is not the "final answer" in water-quality methodology, but it does represent a valuable addition to techniques currently used by providing more detailed data regarding the chemistry at the sediment-water interface.

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