Introduction

Background

West Virginia has had a Water Resources Research Institute (WRRI) since the 1960’s. While it has a statewide mandate, it has always been a small program, receiving about $130,000 per year initially and declining gradually to the present $80,000. Between 1996 and 1999, there was no state WRRI program as all of the research projects were funneled through regional review committees.

Starting last year, the research program came back to the states and this year, for the first time in memory, the amount of research dollars was increased. With water related issues increasing in importance to the state, this is the time to re-invigorate the West Virginia Water Resources Research Institute (WRRI).

Objective

The objective is to make the WRRI the premier water research center in West Virginia and, within selected fields, an international leader.

Strategy

West Virginia has the National Mine Land Reclamation Center, a large, self-sustaining, internationally recognized program which focuses on water issues: acid mine drainage and coal combustion byproducts. West Virginia also has the Institute for Industrial Decommissioning which develops environmentally safe methods for industrial site and other brownfields remediation. While each of these programs is well known within their specific technical fields, they have had no single coordinating body and no common identity. On the other hand, at $80,000 per year, the West Virginia WRRI will never be a significant research program. The proposed strategy is to make WRRI the coordinating body for all of these programs and employ the State Advisory Committee for Water Research as the overall advisory body.

In addition, the West Virginia WRRI has contacted Marshall University requesting they explore, with WVU, ways in which their water research programs be integrated within the State’s WRRI framework.

Priorities for FY 2002

Coal Mining: Reforestation, watershed protection and remediation, abandoned mine lands, stream habitat classification, acid mine drainage, habitat fragmentation. Manufacturing: Brownfield site cleanup technology, standards development, economic and environmental impact analysis. Agriculture: Combined animal feeding operations, nutrient and pathogen impacts on streams, aquaculture, pollutant source identification. Forestry: Stream sedimentation targets and monitoring procedures, road construction and reclamation practices. Electric Power Generation: Volatile mercury emissions, coal combustion product use and disposal, carbon dioxide production/sequestration.
Membership of the West Virginia Advisory Committee for Water Research (as of January 8, 2001)

Members:

Benjamin Greene, Chairman West Virginia Coal Association

Mike Castle, Director West Virginia Division of Environmental Protection

Roger Calhoun, Head USDI, Office of Surface Mining, Charleston Field Office

Ron Evaldi, Hydrologist USGS, West Virginia Division

Paul Dunn, Assistant State Conservationist USDA, Natural Resources Conservation Service

Sam Lockard, Natural Resources Coordinator West Virginia Farm Bureau, Inc.

Invited:

Gary Bryant, Environmental Engineer U.S. EPA, Region III

Carl Bauer, Associate Director for Coal and Environmental Systems U.S. DOE/National Energy Technology Laboratory

Rick Herd, Water Resources Manager Allegheny Energy, Inc.

Kiena Smith, Executive Director Canaan Valley Institute

David Meadows, Chief, Environmental and Remediation Section U.S. ACE/Huntington District

Accomplishments

Policy initiatives which were developed with the assistance of the West Virginia Water Resources Research Institute:

Appalachian Clean Streams Initiative (ACSI)

For decades, the problem of stream pollution from acid drainage has been recognized as a major problem in the eastern United States. Over the years, many programs have had great success, but despite the severity of the problem there had not been a coordinated effort with the primary focus of eliminating acid drainage until the Appalachian Clean Streams Initiative was introduced in the fall of 1994.

In early 1994, representatives of USDI/OSM and the West Virginia Water Resources Research Institute’s National Mine Land Reclamation Center met to develop methods for focusing resources and technology on remediating watersheds damaged by acid mine drainage. The result was the Appalachian Clean Streams Initiative as adopted by Director Robert Uram in November of that year. The strategy involved development of grass roots watershed organizations, partnerships with state programs and the industry. The program has received increasing funding from Congress ($11m in the current year), has resulted in implementation of innovative technology, the cleanup of acid mine drainage in numerous streams and has helped nurture the watershed movement in the participating states. The West Virginina WRRI remains an integral part of ACSI providing technical support to states and watershed organizations through an annual contract provided by USDI/OSMRE.
The Appalachian Clean Streams Initiative began as a broad-based program to eliminate acid drainage from abandoned coal mines. Today the program is more focused, with a clear goal of cleaning up acid drainage problems using a combination of private and government resources.

The mission of the Appalachian Clean Streams Initiative is to facilitate and coordinate citizen groups, university researchers, the coal industry, corporations, the environmental community, and local, state, and federal government agencies that are involved in cleaning up streams polluted by acid drainage. The initiative responds to all major interests in this endeavor. Although eliminating acid drainage is now a federal government priority, the problem is so widespread and costly to solve that it can be eliminated only through combined public and private efforts.

The Appalachian Clean Streams Initiative is an opportunity for a partnership to solve one of the major environmental problems facing the regional ecosystems of the coalfields. The major benefits of coordinating acid drainage cleanup are:

Environmental Clean-up - Acid drainage has a devastating impact on people’s lives and the vitality of the local economy. The benefits of cleaning up the rivers and streams can be observed and measured, and coordinated success produces significant long-term benefits.

Multi-agency Coordination - An outcome-oriented approach focuses a host of new talent and resources from traditional research organizations on projects that promise enhanced quality of life and health for the public. State, local, and community expertise and knowledge synergize as government and private groups work together to address a common problem.

Reinventing Government - This is an excellent opportunity to test the reinventing government principle of doing more with less. Interagency coordination will result in better use of public money and government personnel in a way that responds to the needs of the people affected by acid drainage.

Benefits for Local Economies - Clean-up of acid drainage will promote tourism and recreational activities, including hiking, camping, fishing, and boating.

Ecosystem Approach - This plan for eliminating acid drainage is based on cleaning up watersheds, an approach that helps ensure funds are wisely spent. In addition, cleaning up the watersheds provides an opportunity for native plants and animals to once again inhabit the watersheds.

Citizen and Corporate Involvement - A critical aspect of the Appalachian Clean Streams Initiative is meeting the needs of the coalfield residents and involving the people who live in the coal fields and gaining the support of corporations including those in the coal industry. By combining their resources, they can help ensure that clean-up efforts bring about tangible benefits to people and the environment.

West Virginia Coal Ash Policy

In 1997 the West Virginia Division of Environmental Protection’s (DEP), Office of Mining and Reclamation (OMR) recognized the need for guidance to the mining, utility and manufacturing industries on the beneficial use of coal combustion byproducts (CCB’s). The OMR further recognized that CCB’s have both beneficial uses and the potential to provide positive impacts when properly managed. The West Virginia Coal Ash Policy, developed with the assistance of the West Virginia Water Resources Research Institute, provides the necessary guidance and required criteria for the beneficial use of coal combustion byproducts regulated under State statute so long as such placement is in conformance with an approved plan or permit issued pursuant to such provisions of the code.
The West Virginia Coal Ash Policy recognizes specific beneficial uses for CCB’s and includes guidance as to amounts deemed beneficial under specific geological settings. The Director of the West Virginia WRRI worked closely with the OMR in developing this guidance and developed the formula (imbedded in the policy) by which such amounts are calculated.

The West Virginia WRRI funding also provided initial support for the following programs which are currently in use within West Virginia and other state programs:

1. Methods to value changes in acid related water quality parameters for ecreational fishermen in the Monongahela Forest and recreational boaters and white water rafters on the Cheat River. These methods are presently in use by the West Virginia Department of Natural Resources.

2. The development of the Natural Resource Analysis Center (NRAC) in the College of Forestry, Agriculture and Consumer Science. NRAC is now a recognized center for applications of GIS, remote sensing, and related technologies to environmental and natural resource management in West Virginia and Appalachia. NRAC now works with a variety of state and federal agencies, non-profit organizations, and local citizen groups to understand environmental and natural resource management questions.

3. Continued development of the Watershed Characterization and Modeling System (WCMS) now used by various offices in the West Virginia Division of Environmental Protection and currently under development for the Maryland Bureau of Mines to support permitting and management activities.

Research Program

West Virginia WRRI projects completed during FY2000 include the following:

WRI27 - Arsenate Sorption to Actively Treated Acid Mine Drainage Sludge Start Date: 3/1/99 End Date: 2/28/01 WRI30 - Nutrient Impacts on Macroinvertebrates and Periphyton Community Structures Start Date: 3/1/00 End Date: 2/28/01 WRI31 - AMD Models for TMDL Development and Implementation Start Date: 3/1/00 End Date: 2/28/01 WRI32 - WV WRRI Information Transfer Start Date: 3/1/00 End Date: 2/28/01

The following WV WRRI projects are currently underway:

WRI24 - Enhanced Decision Support for TMDL’s Start Date: 7/17/00 End Date: 9/28/01 WRI39 - Water Quality Measurement in Polishing Ponds Start Date: 4/1/01 End Date: 3/31/03 WRI40 - Aquaculture Waste Control & Optimizing Nutrient Utilization Start Date: 4/1/01 End Date: 3/31/03

The following WV WRRI project is pending:

WRI38 - Long Term Effects of Coal Mining on Streams in the Appalachian Region Start Date: 9/1/01 End Date: 8/31/03

Information on the completed projects are included in this annual report. For more information on currently on-going or pending projects, contact:

Paul F. Ziemkiewicz, Director West Virginia Water Research Institute West Virginia University PO Box 6064 Morgantown, WV 26506-6064 (304) 293-2867 x 5441 pziemkie@wvu.edu
Basic Information

<table>
<thead>
<tr>
<th><strong>Title:</strong></th>
<th>Arsenate Sorption to Actively Treated Acid Mine Drainage Sludge</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Project Number:</strong></td>
<td>WRI27</td>
</tr>
<tr>
<td><strong>Start Date:</strong></td>
<td>3/1/1999</td>
</tr>
<tr>
<td><strong>End Date:</strong></td>
<td>2/28/2001</td>
</tr>
<tr>
<td><strong>Research Category:</strong></td>
<td>Water Quality</td>
</tr>
<tr>
<td><strong>Focus Category:</strong></td>
<td>Water Quality, Treatment, Geochemical Processes</td>
</tr>
<tr>
<td><strong>Descriptors:</strong></td>
<td>acid mine drainage, aresenate, sulfate, zero point of charge</td>
</tr>
<tr>
<td><strong>Lead Institute:</strong></td>
<td>West Virginia University</td>
</tr>
<tr>
<td><strong>Principal Investigators:</strong></td>
<td>Louis M. McDonald, Louis M. McDonald</td>
</tr>
</tbody>
</table>

Publication
Problem and Research Objectives

In an active mine drainage treatment system, metal and proton acidity is neutralized by the continuous addition of a base like NaOH or NH₃. Iron is frequently the metal present in the largest concentration and so one product of neutralization is an amorphous iron hydroxide sludge. These sludges are concentrated in settling ponds, and the overlying water discharged into nearby waterways. Discharged water must meet regulatory effluent limits for metals, pH and any other parameters that may be of concern.

One contaminant of concern is arsenic (As). Arsenic is a toxic element that has been in the news recently because of a proposal to reduce the current water quality standard of 50 ppb to 10 ppb. In neutralized acid mine drainage, arsenic can precipitate or co-precipitate as a solid, bind to the surface of a mineral like iron oxide or hydroxide (sorption), and it can remain dissolved to be discharged. Because iron oxides are good scavengers for oxyanions such as phosphate (PO₄³⁻), sulfate (SO₄²⁻), and arsenate (AsO₄³⁻), sorption is an important mechanism for arsenic removal from solution.

The potential for iron oxides to sorb a contaminant ion like arsenate from solution is dependent on solution pH and the presence of competing ions. In acid solutions, oxides surfaces have a net positive charge and anion sorption is favored by electrostatic attraction. As solution pH increases, net positive charge decreases and at some point becomes zero. As solution pH increases past the zero point of charge, net charge on the oxide becomes negative. The zero point of charge for amorphous and crystalline iron oxides is typically between 7 and 9. The ion in mine drainage most likely to compete with arsenate for sorption sites is sulfate because the sulfate concentrations of mine drainages can be several orders of magnitude higher than arsenate concentrations. There are two principal mechanisms by which sulfate might hinder arsenate sorption to acid mine drainage sludge. First, sulfate might compete with arsenate for surface sorption sites. Second, specific sulfate sorption would increase the negative charge on the sludge surface and therefore repel the negatively charged arsenate ion. In either case, the effect is to increase dissolved arsenate concentrations.

Our objective was to determine the effect of sulfate on arsenate sorption to acid mine drainage sludge at the neutralization pHs of a typical active treatment process.

Principal Findings and Significance

Physico-chemical properties of AMD sludge

Acid mine drainage sludge was prepared by neutralizing 1mM (56 mg L⁻¹) iron (Fe) solutions containing either 0, 2.5 or 5.0 mM SO₄ (0, 240, and 480 mg
SO$_4$ L$^{-1}$) to pH 7, 8 or 9 (3 x 3 factorial) with sodium hydroxide. Settled sludge volume was determined after 1 hr using an Imhoff cone, settled sludge mass was determined gravimetrically. Sludge mass was significantly lower at pH 8 and 9 compared to pH 7 (Figure 1), and was higher in 5 mM SO$_4$ than at 0 or 2.5 mM SO$_4$ (Figure 2). Settled sludge volumes decreased linearly with increasing pH (Figure 1) and were smaller when sulfate was present (Figure 2).

![Figure 1. Effect of neutralization pH on the mass and volume of sludge settled from one liter of 1 mM Fe solution.](image)

The zero point of charge of freshly precipitated acid mine drainage sludge as a function of sulfate concentration was determined using a cation exchange, anion exchange capacity technique. The zero point of charge of sludge neutralized with sodium hydroxide was 7.6 and did not change when the sulfate concentration was increased from 0 to 2.5 to 5.0 mM at fixed iron concentration of 1 mM. This suggests that sulfate is not specifically sorbing to the sludge surface.

**Arsenate sorption to AMD Sludge**

There was a significant effect of initial As concentration on the percent As removed from solution (Figure 3). Whereas 99% of the initial As was removed from the 5.3 mg L$^{-1}$ As treatment, only 84% was removed from the 25 mg L$^{-1}$ As treatment. This represents a dissolved As concentration of 53 µg L$^{-1}$ for the 5.3 mg L$^{-1}$ arsenic treatment, and 4.0 mg L$^{-1}$ for the 25 mg L$^{-1}$ arsenic treatment.
Figure 2. Effect of sulfate concentration on the mass and volume of sludge settled from one liter of 1 mM Fe solution.

Figure 3. Effect of initial arsenate concentration on the % arsenate removed from solution. Columns labeled with different letters indicate treatments significantly different ($\alpha=0.05$).
To account for the effect of neutralization pH and sulfate concentration on the mass of precipitated sludge, arsenate sorption was calculated as the mass of arsenate removed from solution (mmol) per mass of iron precipitated (mmol). There was a significant trend for arsenate sorption to decrease as pH increased (Figure 4). This observation is consistent with other reports of anion sorption to oxides and hydroxides, and can be explained by the increase in negative charge that develops on variable charge surfaces with increasing pH. Increasing neutralization pH from 7 to 9 decreased arsenate sorption by 28%.

Figure 4. Effect of pH on arsenate sorption. Columns labeled with different letters indicate significantly different (α=0.05).

Sulfate at the highest concentration significantly decreased percent As removed from solution (Figure 5). There were no differences between the 0 and 2.5 mM SO\textsubscript{4} treatments. A sulfate-to-arsenate ratio of 15:1 decreased arsenate sorption by 5.2%. Although sulfate at high concentrations can significantly reduce arsenate sorption, the effect is quantitatively less important than the effect of neutralization pH.

There three principal conclusions from this work are,
1. Sulfate did not specifically sorb to acid mine drainage sludge surfaces. This result has implications for the sorption of contaminant cations and anions. Sulfate does have an effect on the settled mass and volume of active treatment sludge.
2. Sulfate does interfere with arsenic sorption but the effects are small relative to the effects of neutralization pH, at least when neutralization pH is between 7 and 9.

3. The trend for arsenic sorption to increase as pH decreases suggests that active treatment systems designed to remove metals, acidity and arsenic should do so in a two-stage treatment process. This will be particularly critical for drainages where manganese is to be removed as well.

![Graph showing arsenic adsorption vs sulfate concentration](image)

Figure 5. Effect of sulfate concentration on arsenate sorption. Columns labeled with different letters indicate significant difference ($\alpha=0.05$).

Descriptors: acid mine drainage, arsenate, sulfate, zero point of charge

Awards and Achievements: none to date. A peer-reviewed journal article is planned.

Information Transfer Program: none

Student Support: none
Basic Information

<table>
<thead>
<tr>
<th>Title:</th>
<th>Nutrient Impacts on Macroinvertebrate and Periphyton Community Structure</th>
</tr>
</thead>
<tbody>
<tr>
<td>Project Number:</td>
<td>WR130</td>
</tr>
<tr>
<td>Start Date:</td>
<td>3/1/2000</td>
</tr>
<tr>
<td>End Date:</td>
<td>2/28/2001</td>
</tr>
<tr>
<td>Research Category:</td>
<td>Biological Sciences</td>
</tr>
<tr>
<td>Focus Category:</td>
<td>Nutrients, Non Point Pollution, Water Quality</td>
</tr>
<tr>
<td>Descriptors:</td>
<td>nutrients, animal waste, periphyton, benthic macroinvertebrates, non-point pollution, agriculture, poultry</td>
</tr>
<tr>
<td>Lead Institute:</td>
<td>West Virginia University</td>
</tr>
<tr>
<td>Principal Investigators:</td>
<td>Peter Benjamin Vila, Neil Gillies</td>
</tr>
</tbody>
</table>

Publication
Final Project Report for WRRI

**Title:** Nutrient Impacts on Macroinvertebrate and Periphyton Community Structure.

**Duration:** March 2000 to February 2001.

**Principal Investigators:** Dr. Peter Vila, Shepherd College  
W. Neil Gillies, Cacapon Institute
Problem and Research Objectives

Agriculture, led by the integrated poultry industry and beef cattle production, is a key element in the West Virginia Potomac Headwater regions economy. The rapid expansion of the poultry and beef production in this region beginning in the early 1990's has raised concerns over the potential water quality problems caused by this industry.

This project will provide critical data in high gradient streams on the effects of nutrients on the plant periphyton and animal macroinvertebrate community. The watersheds selected for study in the eastern panhandle of West Virginia have small, mostly scattered human habitation with only a few small towns and no point source industry. The Lost River watershed is characterized by a high density of poultry houses and associated agricultural production (row crops, beef cattle); the North River watershed is similar in overall land use to the Lost, with the major difference being a much lower intensity of agricultural production.

Funded activities under the WVWRRI grant include:

- Collection and analysis of periphyton community data
- Analysis of sediment nutrient load
- Analysis of the macroinvertebrate community data collected by WVDEP.

The goal of these studies was to provide a comprehensive picture of the relationship between nutrients, periphyton and benthic macroinvertebrates, and physical characteristics in a high priority watershed impacted by intense agriculture, and in a watershed with lower agricultural impacts.

Principal Findings and Significance
(Tabular results of correlation analysis in Appendix A)

Periphyton

Periphyton metrics were significantly correlated with both land use and water quality parameters. Taxa tolerant to organic enrichment tended to be more abundant in sites likely to be enriched (as indicated by percent land in Row Crop and by high nitrate concentrations). Conversely, taxa sensitive to organic pollution were less abundant in these areas. Indicators of periphyton diversity (e.g., Total periphyton taxa and Total periphyton diversity) tended to increase along with percent Land in Row Crop and poultry house density.

The diatom Achnanthes minutissima was particularly useful as an indicator of low phosphorus levels and was more dominant in sites with low median phosphorus levels. Periphyton biomass tended to increase along with the number of poultry houses and mean total phosphorus levels. Periphyton biomass did not increase with amount of land in row crop or
with mean total nitrate levels. However, periphyton biomass did not correlate with median total phosphorus levels.

Median total phosphorus influenced periphyton diversity, and, along with nitrate, varied inversely with the periphyton Pollution Tolerance Index. Correlations of periphyton metrics to phosphorus concentrations were unexpected. In-stream phosphorus levels in these watersheds (unlike nitrate) are mostly quite low and do not differ greatly between sites. Thus, these results demonstrate the sensitivity of periphyton metrics to very small differences in phosphorus concentrations.

**Sediment nutrient load**

There were large within site differences in sediment nutrient concentrations. This large variability resulted in no significant correlations between any periphyton index and sediment nutrient load.

**Macroinvertebrate community data**

With the exception of number of EPT (Ephemeroptera, Plecoptera, Trichoptera) taxa, benthic invertebrate metrics were mostly unrelated to either land use and nutrient water quality. The number of EPT taxa decreased with increasing intensity of agricultural land use (percent of land in agriculture, row crop, and poultry houses) and nitrate.

Periphyton and diatom diversity showed an inverse relationship with macroinvertebrate indexes and community structure. As the number of periphyton and diatom taxa increased, dominance in the benthic invertebrate community also increased, while the % Chironomids, number of taxa, and number of EPT taxa decreased.

**Significance of findings**

The results indicate that periphyton community metrics and biomass have the potential to serve as sensitive indicators of the nutrient conditions in streams and may serve as surrogates for “measuring” the often ephemeral nutrient loads associated with non-point source pollutants. Periphyton may prove to be an important tool in the development and implementation of nutrient standards designed to protect ecosystem health.

Overall, with the exception of the EPT metric, benthic macroinvertebrate community metrics showed little sensitivity to either nutrients or land use. This may limit their applicability for use in assessing the condition of streams primarily impacted by non-point source nutrient pollution.
Descriptors: Nutrients, animal waste, periphyton, benthic macroinvertebrates, non-point pollution, agriculture, poultry

Awards and Achievements: None.

Articles in Referred Scientific Journals: None. Publications in progress.

Book Chapters: None.

Dissertations: None.

Water Resources Research Institute Reports: None.


Other Publications: Publications detailing results and applications are in progress.

Any other Notable Achievements and Awards: None.

Information Transfer Program: Not applicable.

Student Support: This grant has provided a unique opportunity for internship training. Two student interns worked with the principal investigators in all aspects of the study. This allowed them training in impact assessment, project development, field and laboratory data collection and analysis, and data summary.
Appendix A: Results of correlation analysis on nutrient, land-use, periphyton and benthic macroinvertebrate data.

**Correlations with Land Use**

The Percentage of land in row crop was the land use with the largest number of correlations to various periphyton and benthic invert metrics and water quality.

**As the Percentage of Land in Row Crop Increased**

<table>
<thead>
<tr>
<th>These metrics increased</th>
<th>These metrics decreased</th>
</tr>
</thead>
<tbody>
<tr>
<td>% Motile Diatoms (r=0.76)</td>
<td># EPT Taxa (r=-0.66)</td>
</tr>
<tr>
<td>% Tolerant Diatom Taxa (r=0.75)</td>
<td>% Sensitive Diatom Taxa (r=-0.59)</td>
</tr>
<tr>
<td># Motile Diatoms (r=0.68)</td>
<td>% A. minutissima (r=-0.54)</td>
</tr>
<tr>
<td>Total Periphyton Taxa (r=0.61)</td>
<td></td>
</tr>
<tr>
<td>Total Chlorophyta Cells (r=0.61)</td>
<td></td>
</tr>
<tr>
<td># Chlorophyta Taxa (r=0.56)</td>
<td></td>
</tr>
<tr>
<td>Total Periphyton Diversity (r=0.44)</td>
<td></td>
</tr>
<tr>
<td>Diatom Diversity (r=0.44)</td>
<td></td>
</tr>
</tbody>
</table>

**Water Quality Parameters**

| Maximum NO$_3$-N (r=0.70) |
| Mean NO$_3$-N (r=0.66) |
| Median Total P (r=0.65) |
| Median PO$_4$-P (r=0.47) |

**As the Drainage Area of Sites Increased**

<table>
<thead>
<tr>
<th>These metrics increased</th>
<th>These metrics decreased</th>
</tr>
</thead>
<tbody>
<tr>
<td>Periphyton Taxa (r=0.53)</td>
<td>% Chironomids (r=-0.55)</td>
</tr>
</tbody>
</table>

**As the % of Land in Agriculture Increased**

<table>
<thead>
<tr>
<th>These metrics increased</th>
<th>These metrics decreased</th>
</tr>
</thead>
<tbody>
<tr>
<td>Max NO3-N (r=0.41)</td>
<td># EPT Taxa (r=-0.48)</td>
</tr>
</tbody>
</table>
Correlations with Land Use (continued)

The Number Of Poultry Houses per Square Mile was significantly correlated to various periphyton and benthic invertebrate metrics and water quality.

As the # Of Poultry Houses per Sq. Mi. Increased

<table>
<thead>
<tr>
<th>These metrics increased</th>
<th>These metrics decreased</th>
</tr>
</thead>
<tbody>
<tr>
<td>Periphyton Dry Mass (r=0.79)</td>
<td># EPT Taxa (r=-0.44)</td>
</tr>
<tr>
<td>Periphyton Ash Free Dry Mass (r=0.78)</td>
<td></td>
</tr>
<tr>
<td>Periphyton Chloro-a (r=0.77)</td>
<td></td>
</tr>
<tr>
<td>% Motile Diatoms (r=0.54)</td>
<td></td>
</tr>
<tr>
<td>Periphyton Autotrophic Index (r=0.54)</td>
<td></td>
</tr>
<tr>
<td>Diatom Diversity (r=0.48)</td>
<td></td>
</tr>
<tr>
<td># Diatom Taxa (r=0.44)</td>
<td></td>
</tr>
</tbody>
</table>

Water Quality Parameters

| Mean Total P (r=0.74) |             |
| Mean Turbidity (NTU) (r=0.66) |             |

Correlations with Water Quality

As Mean NO₃-N concentrations Increased

<table>
<thead>
<tr>
<th>These bio-metrics increased</th>
<th>These bio-metrics decreased</th>
</tr>
</thead>
<tbody>
<tr>
<td>% Tolerant Diatoms (r=0.79)</td>
<td># EPT Taxa (r=-0.53)</td>
</tr>
<tr>
<td>Periphyton Poll. Tol. Index (r=-0.50)</td>
<td></td>
</tr>
<tr>
<td>% Sensitive Diatoms (r=-0.48)</td>
<td></td>
</tr>
</tbody>
</table>

As Maximum NO₃-N concentrations Increased
<table>
<thead>
<tr>
<th>These bio-metrics increased</th>
<th>These bio-metrics decreased</th>
</tr>
</thead>
<tbody>
<tr>
<td># Motile Diatoms ($r=0.85$)</td>
<td>Periphyton Poll. Tol. Index ($r=-0.49$)</td>
</tr>
<tr>
<td>% Motile Diatoms ($r=0.67$)</td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>As Mean Total Phosphorus concentrations Increased</th>
</tr>
</thead>
<tbody>
<tr>
<td>These bio-metrics increased</td>
</tr>
<tr>
<td>-----------------------------</td>
</tr>
<tr>
<td>Periphyton Dry Mass ($r=0.57$)</td>
</tr>
<tr>
<td>Periphyton Ash Free DM ($r=0.55$)</td>
</tr>
<tr>
<td>Periphyton Autotroph Index ($r=0.45$)</td>
</tr>
<tr>
<td>Periphyton Chloro-a ($r=0.43$)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>As Median Total Phosphorus concentrations Increased</th>
</tr>
</thead>
<tbody>
<tr>
<td>These bio-metrics increased</td>
</tr>
<tr>
<td>-----------------------------</td>
</tr>
<tr>
<td>% Motile Diatoms ($r=0.61$)</td>
</tr>
<tr>
<td>Tot Periphyton Diversity ($r=0.52$)</td>
</tr>
<tr>
<td># Motile Diatoms ($r=0.49$)</td>
</tr>
<tr>
<td>Diatom Diversity ($r=0.48$)</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>As Mean Turbidity Increased</th>
</tr>
</thead>
<tbody>
<tr>
<td>These bio-metrics increased</td>
</tr>
<tr>
<td>-------------------------------</td>
</tr>
<tr>
<td>Periphyton Dry Mass ($r=0.50$)</td>
</tr>
<tr>
<td>Periphyton Ash Free DM ($r=0.48$)</td>
</tr>
<tr>
<td>Periphyton Autotrophic Index ($r=0.45$)</td>
</tr>
</tbody>
</table>

**Correlations with Periphyton Metrics**

<table>
<thead>
<tr>
<th>As the Periphyton Pollution Tolerance Index Increased</th>
</tr>
</thead>
</table>
These bio-metrics increased | These bio-metrics decreased
--- | ---
% *A. minutissima* *(r=0.82)* | % Motile Diatoms *(r=-0.87)*
Diatom Diversity *(r=-0.66)* | 

No correlation to Benthic Invertebrate Metrics

**Correlations with Periphyton Metrics (continued)**

<table>
<thead>
<tr>
<th>As Total Number of Periphyton Taxa Increased</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>These bio-metrics increased</td>
<td>These bio-metrics decreased</td>
</tr>
<tr>
<td>% Dom Benthic Inverts <em>(r=0.59)</em></td>
<td>% Chironomids <em>(r=-0.66)</em></td>
</tr>
<tr>
<td></td>
<td># EPT Taxa <em>(r=-0.57)</em></td>
</tr>
<tr>
<td></td>
<td># Benthic Invert taxa <em>(r=-0.52)</em></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>As Total Number of Diatom Taxa Increased</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>These bio-metrics increased</td>
<td>These bio-metrics decreased</td>
</tr>
<tr>
<td>Periphyton Dry Mass <em>(r=0.60)</em></td>
<td>% Chironomids <em>(r=-0.70)</em></td>
</tr>
<tr>
<td>%2Dom Benthic Inverts <em>(r=0.55)</em></td>
<td># Benthic Invert taxa <em>(r=-0.60)</em></td>
</tr>
<tr>
<td>Periphyton AFDM <em>(r=0.54)</em></td>
<td># EPT Taxa <em>(r=-0.50)</em></td>
</tr>
</tbody>
</table>
### Basic Information

<table>
<thead>
<tr>
<th>Title: AMD Models for TMDL Development and Implementation</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>Project Number: WRI31</td>
<td></td>
</tr>
<tr>
<td>Start Date: 3/1/2000</td>
<td></td>
</tr>
<tr>
<td>End Date: 2/28/2001</td>
<td></td>
</tr>
<tr>
<td>Research Category: Water Quality</td>
<td></td>
</tr>
<tr>
<td>Focus Category: Water Quality, Models, Law, Institutions, and Policy</td>
<td></td>
</tr>
<tr>
<td>Descriptors: AMD, TMDL, water quality modeling, GIS, environmental policy</td>
<td></td>
</tr>
<tr>
<td>Lead Institute: West Virginia University</td>
<td></td>
</tr>
<tr>
<td>Principal Investigators: Jerald Fletcher</td>
<td></td>
</tr>
</tbody>
</table>

### Publication
WRI31:
AMD MODELS FOR TMDL DEVELOPMENT AND IMPLEMENTATION

FINAL REPORT

Jerald Fletcher, Ph.D.
National Resource Analysis Center
College of Agriculture and Forestry
Division of Resource Management
West Virginia University
Morgantown, WV 26506

James M. Stiles, Ph.D., P.E.
West Virginia Water Resources Institute
West Virginia University
Morgantown, WV 26506
PROBLEM AND RESEARCH OBJECTIVES

A Total Maximum Daily Load (TMDL) assessment is required under section 303 of the US EPA Clean Water Act for all waters that are impaired by pollution. The objective of the TMDL process is to develop an implementation plan whereby impaired waters are systematically returned to health. TMDLs are specific to pollutants. For example, in streams adversely affected by coal mining TMDLs commonly focus on pH and the metal ions: Fe, Mn and Al. Because the transport and reaction of these water quality constituents is rather complex, a computer simulation of these phenomena is required to develop a TMDL for a watershed of any significant size.

This research focused primarily on developing the Total Acidic Mine Drainage Loading (TAMDL) computer program for simulating the stream water quality of watersheds affected by acid mine drainage and its treatment. TAMDL was designed to simulate the stream transport, reaction and loading of temperature, net acidity, pH, dissolved oxygen, ferrous iron, ferric iron, manganese and aluminum. The advection and dispersion terms of the governing equation for these constituents are solved using the explicit McCormack predictor-corrector finite difference method, and the loading and reaction terms are solved with the fourth order Runge-Kutta method. Because TAMDL uses net acidity to model solution buffering, an empirical constitutive relationship is used to calculate stream pH during the simulation.

PRINCIPAL FINDINGS AND SIGNIFICANCE

Governing Equations

The following partial differential equation is solved by TAMDL for each of the water quality constituents, except for proton concentration.

\[
\frac{\partial C_i}{\partial t} = \mu \frac{\partial^2 C_i}{\partial x^2} - V \frac{\partial C_i}{\partial x} + L_i + S_i
\]  

(1)

Where \( C_i \) are the simulated constituents, \( L_i \) are the model node loading terms for each of the constituents and \( S_i \) are the net chemical and physical reaction source (sink) terms for each constituent. The hydrodynamic dispersion, \( \mu \), and the mean stream velocity, \( V \), are simulation parameters. Because these quantities must remain uniform throughout the computational domain, the watershed must be divided into small sub-watersheds before using the computer program. The spatial coordinate, \( x \), proceeds from the head of the sub-watershed and follows the stream channel to the mouth.

The governing equation is solved using net acidity rather than pH. Net acidity includes acidity caused by metal ion hydrolysis as well as by proton acidity (pH). In typical mine drainage, metal ions rather than protons, constitute the major
component of acidity. Therefore, TAMDL estimates pH through its relationship with net acidity by subtracting the effect of the metal ions.

If the governing equation was solved with proton concentration instead of net acidity, then it would be necessary to simulate dissolved carbon dioxide, bicarbonate ion, carbonic acid and total sulfate concentrations in addition to the other constituents. While this would be more pleasing theoretically, each of the additional parameters would require the estimation of boundary and initial conditions, which would degrade overall simulation precision. When net acidity is simulated with the governing equation instead of proton concentration, then a constitutive relationship is required to calculate pH.

The parameter pH must be calculated by the model because water quality standards invariably use pH instead of net acidity and the kinetic rates of ferrous iron, aluminum and manganese oxidation and/or precipitation depend heavily upon pH. The following net acidity – pH constitutive relationship was developed through the empirical examination of pH and net acidity data from samples collected in several small watersheds in West Virginia, Maryland and Pennsylvania (Stiles, Fripp and Ziemkiewicz, 2000).

\[
pH = -\log_{10}[H^+] = a \max\left(1, A^2\right)^{b_{\text{sign}(A)}}
\]

(2)

Where \( A \) is the net acidity of the stream in mg/L CaCO\(_3\) equivalents and \( a, b \) are empirical constants normally calibrated from locally obtained water quality data. If local data is unavailable, \( a, b \) are usually close to 6.5 S.U.-L\(^{2b}/mg^{2b}.CaCO3 \) and –0.02, respectively.

TAMDL assumes that all ferric iron has combined with dissolved oxygen to form ferric oxide. The computer program also assumes that ferric oxide clings to sediment particles in the stream, which leave the computational domain by flowing through the downstream boundary or by sedimentation. The re-suspension of ferric iron containing sediment particles is not simulated by the program. The rate at which ferric iron leaves the model domain via sedimentation is assumed to follow Stokes Law. This assumption is valid when the particle Reynolds number is less than unity (Roberson and Crowe, 1980). Given the size of sediment particles most likely to carry ferric oxide, this assumption is realistic.

The formulation used by TAMDL to calculate the kinetic rate of manganese oxidation and precipitation was obtained from Stumm and Morgan (1981). When the stream’s dissolved oxygen concentration is less than 0.01 mg/L, manganese oxidation and reduction are neglected.

\[
\text{Mn}^{2+} + \text{H}_2\text{O} + \frac{1}{2}\text{O}_2 \rightarrow \text{MnO}_2 + 2\text{H}^+ \]

(3)
The kinetic rate for the progress of manganese oxidation and precipitation, \( S'_{Mn} \) is calculated by the program using the following formula. The array containing the net rate of production (consumption) for each of the constituents, \( S_i \) is calculated by taking the algebraic sum of the kinetic rates for each chemical and physical reaction being modeled. Because manganese oxidation and reduction consumes oxygen, equation (3) is used to calculate the corresponding decline in dissolved oxygen concentration. The effect of this reaction’s proton production on the pH and net acidity is calculated with equation (3) and the net acidity – pH constitutive relationship.

\[
S'_{Mn} = \frac{-a_{Mn}C_{Mn}C_{DO}C_{Fe3+}}{[H^+]^2} \exp\left(\frac{-E_{Mn}}{RT}\right)
\]

Where \( E_{Mn} \) is an empirical rate constant assumed by the program to be 107.987 kJ/mole, \( a_{Mn} \) is an empirical rate multiplier specified by the user with units of L\(^4\)/\((\text{mg}^4 \cdot \text{day}) \) and \( R \) is the universal gas constant, 8.314 x 10\(^-3\) kJ/mole/K. The stream water temperature, \( T \), must be in K, \( C_{Mn} \) is the manganese concentration, \( C_{DO} \) is the stream’s dissolved oxygen concentration and \( C_{Fe3+} \) is the ferric iron concentration. All of the concentrations in equation (4) are in mg/L.

The chemical reaction for aluminum precipitation is similar to the equation for manganese oxidation and precipitation except for the absence of oxidation because aluminum has only a single oxidation state.

\[
\text{Al}^{3+} + 3\text{H}_2\text{O} \rightarrow \text{Al(OH)}_3 + 3\text{H}^+
\]

\[
S'_{Al} = \frac{-a_{Al}C_{Al}A_{Al}}{[H^+]^3} \exp\left(\frac{-E_{Al}}{RT}\right)
\]

Where \( S'_{Al} \) is the kinetic rate for aluminum precipitation, equation (5), \( a_{Al} \) is the dimensionless empirical rate constant specified by the user, \( C_{Al} \) is the aluminum concentration in mg/L and \( A_{Al} \) is the empirical rate multiplier assumed by TAMDL to be 3160 mole\(^3\)/L\(^3\)/day. The other empirical rate constant, \( E_{Al} \), is assumed by the program to be 58.2 kJ/mole. Like for manganese precipitation and oxidation, the effect of this reaction’s production of protons on the pH and the net acidity is calculated with equation (5) and the net acidity – pH constitutive relationship.

If the user specifies a negative value for the dimensionless empirical rate constant, \( a_{Al} \), the program does not evaluate equation (6), but does not allow the aluminum concentration to be greater than the solubility limit under equilibrium conditions, \( C_{Al\text{-equ}} \) which is calculated with equation (7).

\[
C_{Al\text{-equ}} = \exp(35.071 - 6.9078 \text{pH})
\]
While not necessary for the application that will be discussed in this paper, ferrous iron oxidation can be simulated by TAMDL with the following chemical reaction. When the stream's dissolved oxygen concentration is less than 0.01 mg/L, ferrous iron oxidation is neglected.

\[
\text{Fe}^{2+} + \frac{1}{4} \text{O}_2 + \frac{5}{2} \text{H}_2\text{O} \rightarrow \text{Fe(OH)}_3 + 2\text{H}^+ \tag{8}
\]

The rate of ferrous oxidation, \(S'_{\text{Fe}^{2+}}\), is calculated by the program with the formulation presented by Kirby, Thomas, Southam and Donald (1998). This formulation has a biotic term as well as an abiotic term to account for the oxidation of ferrous iron by *T. ferrooxidans* bacteria.

\[
S'_{\text{Fe}^{2+}} = - U_{\text{DO}} A_a C_{\text{Fe}^{2+}} C_{\text{DO}} \exp\left(-\frac{E_a}{RT}\right) - U_{\text{DO}} A_b C_{\text{Fe}^{2+}} C_{\text{DO}} C_{\text{TF}} [\text{H}^+] \exp\left(-\frac{E_b}{RT}\right) \tag{9}
\]

Where \(U_{\text{DO}}\) converts equation (9) from the units used by Kirby, Thomas, Southam and Donald (1998) to the units employed by TAMDL and is 3.125117192 \times 10^{-5} \text{ g-moles O}_2 / \text{ mg O}_2. The empirical abiotic oxidation rate multiplier, \(A_a\), is 3.456 \times 10^{10} \text{ mole/L/day}, and the empirical abiotic rate constant, \(E_a\), is 96 kJ/mole. The ferrous iron concentration in mg/L is \(C_{\text{Fe}^{2+}}\), and the dry biomass concentration of *T. ferrooxidans* bacteria is \(C_{\text{TF}}\). The empirical biotic rate constants, \(A_b\) and \(E_b\), are 8.8128 \times 10^{13} \text{ mole/L/day} and 58.77 kJ/mole, respectively. All of the empirical rate constants in equation (9) were determined from the analysis of field data (Kirby, Thomas, Southam and Donald, 1998).

Because the kinetic rates of manganese oxidation and precipitation, aluminum precipitation and ferrous oxidation depend upon the stream temperature and the dissolved oxygen concentration, it is necessary that TAMDL simulate these water quality constituents as well. With dissolved oxygen, the user has the option of directing the program to assume that saturated conditions are always present or calculate the dissolved oxygen concentration from stream reaeration and organic material decay. A zeroth order sediment oxygen demand formulation from the lake model *CE-QUAL-W2* (Cole and Buchak, 1995) was adapted for use in TAMDL. Stream reaeration is calculated with the O’Connor and Dobbins (1958) formulation. Because stream temperature is not absolutely crucial to the modeling of streams affected by acid mine drainage, the simplified formulation used by the program assumes that the amount of heat transferred between the stream and the atmosphere is directly proportional to the difference in temperature and wind speed and inversely proportional to the average depth of the stream. The structure of the TAMDL is such that it can easily be modified to read the stream temperatures from the output of a more sophisticated stream temperature model.
Boundary and Initial Conditions

Upstream of the computational domain for each simulation, the user specifies the boundary temperature and concentrations. The specified upstream boundary temperature and concentrations may vary with simulation time. Normally, the upstream boundary condition is calculated from the results of the model for the upstream sub-watershed. If there is no upstream sub-watershed, the upstream boundary condition must be implied from the results of water quality sampling.

At the downstream end of each computational domain, TAMDL assumes that the spatial gradient of the temperature and concentration is zero. Downstream boundary condition required because of the dispersion (second derivative) term in governing equations. If there is no flow through the computational domain, TAMDL automatically applies the downstream boundary condition to the upstream boundary, and the concentrations specified for the upstream boundary are ignored.

The program also requires that the initial temperature and concentration be specified for each node. Initial conditions are not very important when one desires a steady state solution. When one is simulating a transient problem, the precise selection of initial conditions may have an important effect on the results calculated in the early portion of the simulation. Realistic initial conditions can be generated by simulating water quality conditions for a period prior to the desired simulation period.

Numerical Algorithm

Because an Intel based personal computer is normally used to execute TAMDL models, efficient use of computational resources is very important. Therefore, the appropriate numerical algorithm should be both explicit and at least second order accurate in both time and space. One well-tested algorithm that satisfies this requirement is the explicit MacCormack predictor – corrector method described by Anderson, Tannehill and Pletcher (1984). Because this finite difference algorithm is normally applied to the solution of the advection – dispersion equation, the loading and chemical reaction terms in the governing equation must be solved analytically or with a numerical technique for first order ordinary differential equations.

Since the equations describing the kinetic rates of the aforementioned reactions are both complex and non-linear, it was decided that both the loading and reaction terms should be solved numerically. First order ordinary differential equations are commonly solved with one of the Runge-Kutta methods (Boyce and DiPrima, 1977). In order to simplify the program’s source code, it was decided that intermediate time steps to solve the chemical reaction terms would not be employed. Therefore, to achieve the desirable accuracy, it was decided to use the fourth order Runge-Kutta method to solve the contributions of these terms.
**Source Loads**

The source loads applied to one or more finite difference model nodes is represented in TAMDL’s governing partial differential equation, equation (1), by the array $L_i$. The program allows one to specify thermal, alkaline, acid, ferrous iron, ferric iron, manganese, aluminum and dissolved oxygen loads with this array. The operation of passive acid mine drainage treatment systems can also be simulated for specified model nodes. Because the production of alkalinity by passive acid mine drainage treatment systems depend upon the stream’s acidity, the source load terms can be non-linear and the fourth order Runge-Kutta method is also used to calculate the contribution of these terms. When simulating most watersheds for TMDL purposes, only alkaline, acid, ferric iron, manganese and aluminum loads are normally employed.

Most water quality models simulate the transport of constituents whose loading rates are directly proportional to local runoff rates. Because of this proportionality, these models calculate non-point source loads from either precipitation or runoff rates. However, the mine drainage normally has both precipitation driven and non-precipitation driven components and it is normally impossible to generate correlations between precipitation and mine drainage quality or quantity.

**Hydrology**

Because the advection term in the governing partial differential equation, equation (1), contains the mean flow velocity of the stream, $V$, the mean velocity must be known for all portions of the computational domain throughout the simulation period. The current formulation of the explicit MacCormack predictor – corrector method requires that the stream velocity and the hydrodynamic dispersion be uniform throughout the computational domain. Therefore, to account for changes in the stream hydraulics, the watershed must be divided into many small sub-watersheds. Because few watersheds possess the quantity of hydrologic data required to warrant a sophisticated simulation of the stream hydrology and hydraulics, the current version of TAMDL assumes that the flow within each sub-watershed is governed by the Manning’s equation for uniform flow. The program can easily be modified to read the output from a dedicated hydrological simulation package.

**Model Application**

As a part of another research project, the computer program TAMDL was use to create a water quality simulation model of the Paint Creek watershed. Paint Creek, a tributary of the Kanawha River, flows in a northerly direction through parts of Raleigh, Fayette and Kanawha counties in south-central West Virginia (Figure 1) and has a drainage area of 318 km$^2$ (123 mi$^2$). For the past 90 years,
surface and deep coal mines have operated in the watershed. Before the implementation of WVSCMRA and SMCRA, little consideration was given to the environmental degradation that resulted from these activities. Currently, the quality of Paint Creek and its tributaries are being negatively impacted by the acidic drainage from those mines that were abandoned prior to the environmental regulations. The environmental impact of this mine drainage is being manifested in depressed stream pH and elevated concentrations of iron, manganese and aluminum. The ultimate purpose of the modeling effort was to develop a TMDL for these water quality parameters.

Paint Creek watershed was divided into 62 sub-watersheds (Figure 2). The delineation of the watershed was accomplished with the assistance of the Watershed Characterization and Modeling System (WCMS) developed by the National Resource Analysis Center at West Virginia University. The size of these sub-watersheds ranged between 0.10 and 17 km$^2$ (25 and 4,100 acres). While WCMS has the capability to delineate a watershed automatically given a maximum sub-watershed drainage area, certain portions of the watershed required greater resolution because of the greater AMD loading. One portion of the watershed, requiring greater resolution was the area around Ten Mile Fork and Long Branch of Ten Mile Fork (Figure 3).

One of the water quality sample collection stations within the Paint Creek watershed with the best observed data coverage was WVDEP-SRG station number 54 on the Long Branch of Ten Mile Fork (Figure 4). Because of the quantity of data that was available for this station, it is probably the best location within the watershed to illustrate the capabilities of TAMDL. The discharge of Long Branch (Figure 5) was calculated by scaling the observed Coal River discharge measured by the USGS at Tornado, WV according to drainage area. The hydraulic parameters of Long Branch (Table 1) were selected to reflect the hydraulic conditions observed by both WVDEP-SRG and the project investigators. The AMD loading applied to the model above station number 54 (Figure 6) was calculated from the water quality of AML seeps sampled by WVDEP-SRG and adjusted so that the model would replicate observed water quality conditions. The water quality simulation parameters (Table 2) were also adjusted as part of the model calibration process. Because of the scale of the streams simulated by the Paint Creek watershed TAMDL model, the model assumes that all of the iron entering the computational domain is in the ferric oxidation state.

Model Results

The model’s simulation of pH, iron, manganese and aluminum (Figures 7, 8, 9 and 10) show reasonable agreement with the observed data. Of the four water quality parameters, the calculated iron concentration (Figure 8) appears to deviate the most from the observed data. Because the sedimentation of ferric iron is strongly dependent upon the stream hydraulics, this deviation may
indicate that the stream’s hydrology may be in temporal error. Since the model’s stream discharge was calculated by scaling the daily average discharge observed at a stream gage 53 km (33 mi) away from the sub-watershed, the timing of individual storm events are probably in error.

Another way to check the calibration of a water quality model is to compare the cumulative probability distribution functions of the observed and simulated water quality constituent concentrations. The cumulative probability distribution functions of the simulated pH and iron concentration (Figures 11 and 12) show quite reasonable agreement with the distribution functions of the observed data. Unfortunately, the cumulative probability distribution functions for the simulated concentrations of manganese and aluminum (Figures 13 and 14) show significant deviation (approximately 8 and 48 mg/L, respectively) above the 70th percentile. These results suggest either:

1. The observed data set did not adequately define the maximum manganese and aluminum concentrations likely to be observed at the station.
2. Or, the model is underestimating the kinetic rates of equations (3) and (5).
3. Or, the model is overestimating the amount of manganese and aluminum loading during low flow conditions.

While all three of these possibilities are probably true to some extent, the discrepancy in probability distributions underscore the data requirements for successful application of the TAMDL model.

A direct comparison of the simulated and observed pH and metals concentration for station number 54 is given in Table 3. The expected model error magnitude, $S$, was calculated using equation (10).

$$S = \sqrt{\frac{\sum_{i=1}^{n} (C_{i, \text{model}} - C_{i, \text{observed}})^2}{n-1}}$$  \hspace{1cm} (10)

In equation (10), $C_{i, \text{model}}$ is the value of the water quality parameter calculated by the model, $C_{i, \text{observed}}$ is the observed value of the water quality parameter and $n$ is the number of observations.

**Conclusion**

The computer program TAMDL was designed to simulate the stream transport, reaction and loading of temperature, net acidity, pH, dissolved oxygen, ferrous iron, ferric iron, manganese and aluminum. The advection and dispersion terms of the governing equation for these constituents are solved using the explicit McCormack predictor-corrector finite difference method, and the loading and reaction terms are solved with the fourth order Runge-Kutta method. Because
TAMDL uses net acidity to model solution buffering, an empirical relationship is used to calculate stream pH during the simulation. The computer program has demonstrated the ability to simulate the stream water quality of watersheds affected by AMD. Currently the program is being used to construct a pH, iron, aluminum and manganese TMDL model of the Paint Creek watershed. Future applications of the program will include the simulation of in-stream AMD treatment. Future work should be devoted towards increasing the number of water quality constituents that can be simulated and improving the program’s simulation of sub-watershed hydrology.

The WCMS computer program was a useful tool in constructing the Paint Creek watershed TAMDL model. Unfortunately, no connection exists between the two software packages. Indeed, the current structure of WCMS is not very useful in constructing water quality models with any software package outside of WCMS. Some future research effort should be devoted towards changing the structure of WCMS, so that it can generate TAMDL input files automatically from user graphical and tabular input. While WCMS was a useful tool in generating the GIS-type graphics in this report (Figures 1 through 4), much annotation in a graphics editor was required to generate quality figures. No capability exists in WCMS to generate the time series plots required for the other figures in this report. Additional research should be devoted towards changing the structure of WCMS, so that it can automatically generate both time series and GIS-type graphical output from TAMDL’s output files. Given the ability to pre-process and post-process TAMDL input and output, WCMS can then be used by regulatory personnel to develop TMDLs in a timely fashion.

References


DESCRIPTORS

AMD, TMDL, water quality modeling, GIS, environmental policy

AWARDS AND ACHIEVEMENTS

A paper, DEVELOPING MINING TMDL’S WITH TAMD L, which describes the both the theory of the computer program TAMD L and the program’s application to the Paint Creek watershed will be presented at the American Water Resources Association Summer Specialty Conference, Decision Support Systems for Water Resources Management at Snowbird Utah, June 27 – 30, 2001.

INFORMATION TRANSFER PROGRAM

While this research project did not include a formal Information Transfer Program, Dr. Stiles will be teaching a series of short courses in using the computer program TAMD L at West Virginia University in the summer and autumn of 2001. Anticipated attendees will include employees of WVDEP, EPA Region III and other interested parties.

STUDENT SUPPORT

Dr. Stiles received his Doctor of Philosophy Degree in Civil Engineering from the College of Engineering and Mineral Resources at West Virginia University on May 14, 2001 and was partially funded by this project.
### TABLES

#### Table 1. Hydraulic Parameters for Long Branch Sub-watershed.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of Model Nodes</td>
<td>34</td>
</tr>
<tr>
<td>Node Spacing</td>
<td>200.58 m</td>
</tr>
<tr>
<td>Channel Bottom Width</td>
<td>2.00 m</td>
</tr>
<tr>
<td>Channel Inverse Side Slope</td>
<td>2.00 dimensionless</td>
</tr>
<tr>
<td>Channel Bottom Slope</td>
<td>0.0613 dimensionless</td>
</tr>
<tr>
<td>Manning Roughness Coefficient</td>
<td>0.045 dimensionless</td>
</tr>
</tbody>
</table>

#### Table 2. Water Quality Simulation Parameters for Long Branch Sub-watershed.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Maximum Time Step</td>
<td>1.0 days</td>
</tr>
<tr>
<td>Hydrodynamic Dispersion</td>
<td>$9 \times 10^5$ m$^2$/day</td>
</tr>
<tr>
<td>Mean Sediment Particle Diameter</td>
<td>$2 \times 10^{-6}$ m</td>
</tr>
<tr>
<td>Net Acidity - pH Constitutive Relationship Parameter, $a$</td>
<td>6.414215 SU-(L/mg)$^{2b}$</td>
</tr>
<tr>
<td>Net Acidity - pH Constitutive Relationship Parameter, $b$</td>
<td>-0.046430 dimensionless</td>
</tr>
<tr>
<td>Aluminum Precipitation Kinetic Rate Modifier</td>
<td>$10^{-18}$ dimensionless</td>
</tr>
<tr>
<td>Manganese Oxidation and Precipitation Kinetic Rate Modifier</td>
<td>$10^0$ (L/mg)$^4$/day</td>
</tr>
</tbody>
</table>

Table 3. Observed and Simulated Water Quality Data for Station Number 54.

<table>
<thead>
<tr>
<th>Date</th>
<th>Model pH (SU)</th>
<th>Model Iron (mg/L)</th>
<th>Model Manganese (mg/L)</th>
<th>Model Aluminum (mg/L)</th>
<th>Observed pH (SU)</th>
<th>Observed Iron (mg/L)</th>
<th>Observed Manganese (mg/L)</th>
<th>Observed Aluminum (mg/L)</th>
<th>Error Squared pH</th>
<th>Error Squared Iron</th>
<th>Error Squared Manganese</th>
<th>Error Squared Aluminum</th>
</tr>
</thead>
<tbody>
<tr>
<td>07/18/1994</td>
<td>4.4</td>
<td>0.24</td>
<td>1.99</td>
<td>12.53</td>
<td>4.2</td>
<td>0.03</td>
<td>1.84</td>
<td>13.80</td>
<td>0.0518</td>
<td>0.0434</td>
<td>0.0213</td>
<td>1.6157</td>
</tr>
<tr>
<td>01/30/1995</td>
<td>5.5</td>
<td>0.05</td>
<td>0.23</td>
<td>1.61</td>
<td>4.8</td>
<td>0.22</td>
<td>0.39</td>
<td>2.41</td>
<td>0.4560</td>
<td>0.0277</td>
<td>0.0262</td>
<td>0.6357</td>
</tr>
<tr>
<td>06/05/1996</td>
<td>5.1</td>
<td>0.09</td>
<td>0.45</td>
<td>2.97</td>
<td>4.5</td>
<td>0.21</td>
<td>0.62</td>
<td>4.80</td>
<td>0.3722</td>
<td>0.0154</td>
<td>0.0299</td>
<td>3.3387</td>
</tr>
<tr>
<td>07/23/1996</td>
<td>4.5</td>
<td>0.22</td>
<td>1.65</td>
<td>10.44</td>
<td>4.1</td>
<td>0.19</td>
<td>1.41</td>
<td>10.10</td>
<td>0.1648</td>
<td>0.0007</td>
<td>0.0592</td>
<td>0.1127</td>
</tr>
<tr>
<td>08/08/1996</td>
<td>4.2</td>
<td>0.33</td>
<td>3.54</td>
<td>22.22</td>
<td>4.3</td>
<td>0.07</td>
<td>1.64</td>
<td>11.00</td>
<td>0.0115</td>
<td>0.0672</td>
<td>3.6096</td>
<td>125.8323</td>
</tr>
<tr>
<td>09/05/1996</td>
<td>4.3</td>
<td>0.31</td>
<td>3.03</td>
<td>19.16</td>
<td>4.2</td>
<td>0.08</td>
<td>1.79</td>
<td>11.80</td>
<td>0.0027</td>
<td>0.0537</td>
<td>1.5480</td>
<td>54.1049</td>
</tr>
<tr>
<td>10/01/1996</td>
<td>4.9</td>
<td>0.12</td>
<td>0.72</td>
<td>4.66</td>
<td>4.6</td>
<td>0.09</td>
<td>0.83</td>
<td>4.90</td>
<td>0.0774</td>
<td>0.0012</td>
<td>0.0123</td>
<td>0.0596</td>
</tr>
<tr>
<td>01/06/1997</td>
<td>5.0</td>
<td>0.10</td>
<td>0.51</td>
<td>3.38</td>
<td>4.7</td>
<td>0.48</td>
<td>0.54</td>
<td>3.92</td>
<td>0.1168</td>
<td>0.1451</td>
<td>0.0008</td>
<td>0.2950</td>
</tr>
<tr>
<td>11/05/1998</td>
<td>4.3</td>
<td>0.31</td>
<td>2.78</td>
<td>17.28</td>
<td>5.0</td>
<td>0.08</td>
<td>2.00</td>
<td>12.00</td>
<td>0.4509</td>
<td>0.0544</td>
<td>0.6026</td>
<td>27.8932</td>
</tr>
<tr>
<td>03/10/1999</td>
<td>5.6</td>
<td>0.05</td>
<td>0.20</td>
<td>1.42</td>
<td>5.6</td>
<td>0.25</td>
<td>0.16</td>
<td>1.51</td>
<td>0.0000</td>
<td>0.0410</td>
<td>0.0013</td>
<td>0.0087</td>
</tr>
</tbody>
</table>

SSE = 1.7041  \quad S = 0.4  \quad 5.9113  \quad 213.8963
Figure 1. Paint Creek Watershed.
Figure 2. Paint Creek Watershed TAMDL Model Sub-watersheds.
Figure 3. Ten Mile Fork and Long Branch of Ten Mile Fork Sub-watersheds.
Figure 4. WVDEP-SRG Water Quality Sample Collection Station Number 54.
Figure 5. Calculated Stream Discharge for Long Branch of Ten Mile Fork of Paint Creek.
Figure 6. Model AMD loading applied to Long Branch of Ten Mile Fork above WVDEP-SRG Station Number 54.
Figure 7. Simulated and Observed pH for WVDEP-SRG Station Number 54.
Figure 8. Simulated and Observed Iron Concentration for WVDEP-SRG Station Number 54.
Figure 9. Simulated and Observed Manganese Concentration for WVDEP-SRG Station Number 54.
Figure 10. Simulated and Observed Aluminum Concentration for WVDEP-SRG Station Number 54.
Figure 11. Simulated and Observed pH Cumulative Probability Distribution for Station Number 54.
Figure 12. Simulated and Observed Iron Concentration Cumulative Probability Distribution for Station Number 54.
Figure 13. Simulated and Observed Manganese Concentration Cumulative Probability Distribution for Station Number 54.
Figure 14. Simulated and Observed Aluminum Concentration Cumulative Probability Distribution for Station Number 54.
Information Transfer Program

Basic Information

<table>
<thead>
<tr>
<th>Title</th>
<th>WV WRRI Information Transfer</th>
</tr>
</thead>
<tbody>
<tr>
<td>Start Date</td>
<td>3/1/2000</td>
</tr>
<tr>
<td>End Date</td>
<td>2/28/2001</td>
</tr>
<tr>
<td>Descriptors</td>
<td>website, newsletter, workshop, meeting, outreach, dissemination</td>
</tr>
<tr>
<td>Lead Institute</td>
<td>West Virginia University</td>
</tr>
<tr>
<td>Principal Investigators</td>
<td>Paul F. Ziemkiewicz</td>
</tr>
</tbody>
</table>

Publication
Principal Investigator: Paul F. Ziemkiewicz, Director, West Virginia Water Research Institute

State Water Research Organization

The following graphic depicts how the state water research programs are organized within the West Virginia Water Research Institute.

Program:
- National Mine Land Reclamation Center
- Institute for Industrial Decommissioning
- Water Institutes Program
- EPA EPSCoR

Admin. Unit*:
- NRCCE Ziemkiewicz
- NRCCE Black
- NRCCE Vandivort
- WVU/MU Ziemkiewicz/Szwilski (Pending)

FY 2001 Funding:
- $3.0 m
- $1.1M
- 0.70M
- 0.65M

*NRCCE = National Research Center for Coal and Energy
WV WRI Web Site

The West Virginia WRI web site is being completely redeveloped and includes the following information on all WVWRI programs:

- projects
- publications
- events and conference listings
- sponsors/participants
- WRI background
- research priorities
- contacts
- news updates and announcements
- calculators and tools
- links to useful sites

Information on the following WV WRI programs is included within this web site:

- National Mine Land Reclamation Center
- Acid Drainage Technology Initiative
- Appalachian Clean Streams Initiative
- Combustion Byproducts Recycling Consortium
- National Environmental Education Training Center
- Institute for Industrial Decommissioning
- State Water Institutes
- Monongahela Basin Mine Pool Project
- EPA EPSCoR (pending)

In addition, special interest categories are being developed which will include information on the following:

- acid mine drainage
- brownfields
- industrial waste usage
recycling/reuse
rivers and streams
slag
watersheds
bottom ash
fly ash
mine pools
reclamation
remediation
total maximum daily load
water quality

The address for the WV WRI web site is:

http://wvwri.nrcce.wvu.edu

Newsletters & Publications

The web site is expected to be completely developed by September 1, 2001. Thereafter, updates will be made as new information becomes available. Information from the website will be downloadable for use as fact sheets on projects, events, etc. In addition, newsletters such as the Combustion Byproducts Recycling Consortium’s quarterly newsletter, Ashlines, will be downloadable.

Within the ADTI program, the ADTI Prediction Manual was released in April, 2001. This manual is downloadable from the WV WRI web site. Last year’s ADTI manual is also downloadable from the WV WRI web site as are other publications including the final project reports.

Workshops & Meetings

West Virginia Surface Mine Drainage Task Force Symposium
ADTI workshop
April, 2001
Morgantown, West Virginia
The premier meeting for acid mine drainage reclamation techniques in the world. The Task Force was formed by the Governor of West Virginia in 1977 to address issues related to surface coal mining in Appalachia. The West Virginia Water Research Institute normally contributes 2-3 technical papers to the proceedings and WV WRI staff assist in the facilitation and coordination of the symposium.

Abandoned Mine Land Remediation Workshop
US Army Corps of Engineers
November 14-16, 2000
St. Louis, MO
Topics included hard rock and coal mine drainage treatment technologies, design, performance, and cost estimates.

Society of Mine Reclamation Annual Meeting
for State of Indiana regulators, AML staff, and remediation designers
December 4-6, 2000
Jasper, Indiana
Topics of discussion included acid mine drainage control and treatment technologies.

Methods for Measuring and Evaluating the Effects of Mining on Streams: Implications for Underground Coal Development Assessment
West Virginia Water Research Institute
July 25-26, 2001
Morgantown, West Virginia
Technical workshop with invited participants representing experts from industry, state and federal agencies. There will be two background presentations on ground control and mine hydrology followed by three panel sessions.
USGS Summer Intern Program
Student Support

<table>
<thead>
<tr>
<th>Category</th>
<th>Section 104 Base Grant</th>
<th>Section 104 RCGP Award</th>
<th>NIWR-USGS Internship</th>
<th>Supplemental Awards</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>Undergraduate</td>
<td>0</td>
<td>1</td>
<td>2</td>
<td>0</td>
<td>3</td>
</tr>
<tr>
<td>Masters</td>
<td>0</td>
<td>2</td>
<td>0</td>
<td>0</td>
<td>2</td>
</tr>
<tr>
<td>Ph.D.</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Post-Doc.</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Total</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Notable Awards and Achievements
None

Publications from Prior Projects