Stream Water Quality Management:
A Stochastic Mixed-integer Programming Model

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ABSTRACT

Water quality management under the watershed approach of Total Maximum Daily Load (TMDL) programs requires that water quality standards be maintained throughout the year. The main purpose of this research was to develop a methodology that incorporates inter-temporal variations in stream conditions through statistical distributions of pollution loading variables. This was demonstrated through a cost minimization mixed-integer linear programming (MIP) model that maintains the spatial integrity of the watershed problem. Traditional approaches for addressing variability in stream conditions are unlikely to satisfy the assumptions on which these methodologies are founded or are inadequate in addressing the problem correctly when distributions are not normal.

The MIP model solves for the location and the maximum capacity of treatment plants to be built throughout the watershed which will provide the optimal level of treatment throughout the year.

The proposed methodology involves estimation of parameters of the distribution of pollution loading variables from simulated data and use of those parameters to re-generate a suitable number of random observations in the optimization process such that the new data preserve the same distribution parameters. The objective of the empirical model was to minimize costs for implementing pH TMDLs for a watershed by determining the level of treatment required to attain water quality standards under stochastic stream conditions. The output of the model was total minimum costs for treatment and selection of the spatial pattern of the least-cost technologies for treatment. To minimize costs, the model utilized a spatial network of streams in the watershed, which provides opportunities for cost-reduction through trading of pollution among sources and/or least-cost treatment. The results were used to estimate the costs attributable to inter-temporal variations and the costs of different settings for the 'margin of safety'.

The methodology was tested with water quality data for the Paint Creek watershed in West Virginia. The stochastic model included nine streams in the optimal solution. An estimate of inter-temporal variations in stream conditions was calculated by comparing total costs under the stochastic model and a deterministic version of the stochastic model estimated with mean values of the loading variables. It was observed that the deterministic model underestimates total treatment cost by about 45 percent relative to the 97th percentile stochastic model.

Estimates of different margin of safety were calculated by comparing total costs for the 99.9th percentile treatment (instead of an idealistic absolute treatment) with that of the 95th to 99th percentile treatment. The differential costs represent the savings due to the knowledge of the statistical distribution of pollution and an explicit margin of safety. Results indicate that treatment costs are about 7 percent lower when the level of assurance is reduced from 99.9 to 99 percent and 21 percent lower when 95 percent assurance is selected.

The application of the methodology, however, is not limited to the estimation of TMDL implementation costs. For example, it could be utilized to estimate costs of anti-degradation policies for water quality management and other watershed management issues.

Introduction

Water quality management under the US Environmental Protection Agency's (USEPA) watershed approach (USEPA, 2002) incorporates the latest attempts to realize the original goals of the Clean Water Act of 1972 (CWA): to clean-up and protect U.S. waters from both point and non-point sources of pollution. While much progress has been made over the past three decades, 40 percent of the U.S. waters currently do not meet water quality standards, and about half of the nation's 2,149 major watersheds continue to suffer from serious water quality problems (USEPA, 1998).

In the initial years of the CWA, management efforts were primarily limited to at-source control of discharges from individual point sources by requiring use of Best Available Technologies (BAT) under the National Pollutant Discharge Elimination System (NPDES; Section 402 of the CWA 1972). Attention to non-point source discharge control was virtually non-existent because of the perceived relative severity of the problems combined with personnel and budgetary limitations. The complexity in identifying and determining clean-up responsibility was, and remains, a further confounding factor.

The USEPA and other federal agencies have adopted a watershed approach to better integrate non-point sources into the overall water quality management and improvement effort. Simply put, the watershed approach is an attempt to develop a collaborative approach to environmental management that incorporates all stakeholders including the full range of government entities, the private sector, local organizations, and special interest groups. This approach attempts to bring out the best balance among efforts to control point-source pollution and non-point source runoff and to encourage greater public involvement, accountability and progress toward clean water goals. The focus moves away from technology-based point-by-point control to an overall water-quality based approach (USEPA, 1998).

Since watershed level planning allows pollution control by the least-cost methods and sources and thus provides opportunities for pollution trading, it has a promise of cost-savings for implementation of the USEPA's Total Maximum Daily Load (TMDL) program. Both the TMDL program which seeks to bring degraded waters up to current standards and anti-degradation policies designed to protect current water quality levels can benefit from such an integrated approach. Based on a recent U.S. Environmental Protection Agency study, the watershed approach is estimated to reduce TMDL implementation costs by 25-50 percent over the point-by-point source control approach (USEPA, 2001a).

Objectives

This paper presents a methodology that can incorporate economic decisions into the watershed management process as part of an integrated management approach. The approach takes as given the water quality standards and other exogenously determined factors that managers face and develops a portfolio of treatment/management options that accounts for stochastic inter-temporal variations in pollution loads in a watershed into a framework that minimizes treatment costs. The model can be utilized to estimate watershed-based TMDL implementation costs based on the inter-temporal maintenance of water quality standards under a variety of conditions with a specified probability of the 'margin of safety'. It can also be use to estimate costs for anti-degradation policies for water quality management and other watershed management issues.

Motivation

Stream conditions in any watershed constantly change. Water flow as well as pollution levels in streams vary with time and season. Traditional approaches to deal with these types of variability developed a model based on a single observation or the average of a few samples and then performed a sensitivity or scenario analysis on the factors subject to change (Liebman and Lynn, 1966; Loucks et al., 1967; Fletcher et al., 1991; and Phipps et al., 1991, 1992, 1996). In the context of mathematical programming models, the sensitivity analysis amounts to *parametric programming* or *post-optimality analysis* where the model is run again and again while changing the values for some of the variables.

Other approaches that deal with variability with regard to water quality management problems include *chance-constrained programming* (Charnes and Cooper, 1959, 1962, 1963; Sengupta, 1970) and *first-order uncertainty analysis* (Benjamin and Cornell, 1970). In chance-constrained programming the constraints are expected to satisfy the right-hand-side resource vector for a predetermined degree of confidence (Lohani and Thanh, 1978; Zhu et al., 1994). In first-order uncertainty analysis the first two moments of the variable factors are explicitly included in the model (Burges and Lettenmaier, 1975; Burn and McBean, 1985).

What is missing in all these approaches, however, is the explicit consideration of statistical distributions of the variable factors in the model. Shortle (1990) emphasized this point by suggesting that for stochastic emissions, pollution control essentially requires 'improving the distribution of emissions'. Models based on a single observation or mean values do not perform well when distributions of the relevant variables are not normal. Averages or the mean values often hide valuable information. They are biased in the direction of extreme observations if the distribution is skewed. The mean value can be considered as a good representative of the data only if the true distribution is normal. With few exceptions (e.g., Zhu et al., 1994), chance-constrained programming models usually assume normality when the probabilistic constraints are translated into their deterministic equivalents. First-order analysis does not require normality explicitly. However, the first two moments inadequately describe the data if distributions are not symmetric or normal. Higher order moments for many distributions are equally important to modeling accuracy. In the case of water pollution abatement cost comparisons, Shortle (1990) also pointed out that if the mean and variance of the damage function move in the same direction, the covariance between marginal damage and changes in the emissions is negative and abatement is beneficial. However, if the mean and variance move inversely, the sign of the covariance is ambiguous and abatement may not be beneficial. The first-order analysis implicitly assumes zero weight to the higher order moments than the first two.

The US Environmental Protection Agency (USEPA) has adopted a watershed approach to water quality management but continues to require states to promulgate and enforce regulations to maintain water quality standards at all points throughout the year. The implications for these USEPA imperatives for water quality management in a stochastic environment and the inadequacy of traditional stochastic approaches dealing with the non-normal distributions of pollution loading variables were the motivation for developing the stochastic mixed-integer linear programming model presented in this paper.

The General Model

Consider the following stylized description of the watershed management problem. A watershed is defined as the area of land that catches rain and snow and drains or seeps into a common point. Since water always flows downhill, there is a route with a monotonically non-increasing elevation from any point in the watershed to what is called the pour point. Within a watershed, overland flow and/or groundwater discharges combine to form streams that further combine to form larger streams and rivers. The beginning streams are called headwater streams or tributaries, the point where two or more streams join is referred to as node, and the stream reach joining two nodes defines downstream segments. The watershed area can be divided into sub-watersheds or catchments associated with each stream segment. Pollution loading in a tributary can come from non-point or point sources within the catchment's area. Pollution loading in downstream segments can come from either the direct catchments or from the upstream segments that meet at the upstream node.

In any given situation, the specific details of the stream network, the measures of water quality, and the point and non-point sources of pollutant loadings can be quite complex. The models developed to understand the effects of the underlying geology, land composition, and human intervention that lead to elevated pollution levels are often highly non-linear and reflect a wide variety of hydrological, chemical, and biological activities. When remediation efforts are implemented in an attempt to improve water quality, further complexities are introduced. The approach suggested in this model is to impose a simplified approximation to this complex structure which can be used to inform the management or implementation process.

Let y_i^0 (may be a vector composed of different pollutants) denote the initial pollution load in stream segment *i (i* = 1, 2, …, *I)*. This load comes from the exogenous contribution of point and non-point sources (denoted as x_i) within the sub-watershed or catchment area for tributaries. For downstream segments, y_i^0 represent the combination of net contributions of pollution loading from the respective sub-watershed and the initial loading received from upstream segments. Suppose that there are a number of treatment or control technologies indexed by *m* (*m* = 1, 2, …, *M*), which could include point source control and non-point source practices that reduce the pollution load within a given stream segment with associated fixed costs of implementation of $f_{i,m}$ and variable costs for a unit of treatment of $v_{i,m}$. Let $u_{i,m}$ denote the level of treatment by technology *m* utilized within each segment and c_m, if applicable, denote the upper bound on the treatment that can be realized. Note that the stream segment designations are explicitly included to reflect the spatial structure of the watershed problem. Appropriate bounds on the water quality parameters after treatment can also be included as bounds on the post-treatment water quality, y_i.

A mass-balance approach to water quality can be imposed at any point in time by applying a piecewise linear approximation to the vector of outputs from a non-linear water quality model. Inter-temporal variability can be incorporated by modeling the statistical distributions of concentrations and flows that combine to give the pollutant loadings. This involves two steps: (1) determining the distributions and their parameters, and (2) using these parameters to generate observations in a simulation process that can be utilized in further cost minimizing optimization. Let *n* (*n* = 1, 2, …, *N*) further index the draw from the distribution of random loadings with specified parameters used to reflect the stochastic elements of pollution loadings. With this new index, the initial water quality y_i^0 becomes $y_{i,n}^0$, the exogenous contribution of pollution loadings x_i becomes $x_{i,n}$, the decision or choice variable $u_{i,m}$ becomes $u_{i,m,n}$, and the post-treatment water quality y_i becomes $y_{i,n}$.

Although pollution clean-up can be accomplished in a variety of ways such as at-source control, flow-augmentation, isolation of polluted waters, etc., only the issues involved with the option of treatment of polluted watershed are addressed in this paper. Costs for such treatment usually involve two components: a fixed set-up or installation cost and a variable per unit cost of treatment. The presence of fixed costs introduces non-linearity in the cost function. Mathematical programming for this type of 'fixed-charge problems' usually takes the form of a mixed-integer model (MIP), which allows both continuous and discrete (integer) variables. Let $b_{i,m}$ denote the use of technology *m* within segment *i*. If the appropriate objective is to determine the levels of treatment that would meet mandatory water quality standards over a specified flow regime at minimum costs, then a general mixed-integer programming model can be specified using the notation introduced as follows:

$$\text{Minimize} \quad \text{E(cost)} = \underset{\{u_{i,m}\}}{Min} \sum_{i=i}^{I} \sum_{m=1}^{M} \left(f_{i,m} b_{i,m} + v_{i,m} \left(\frac{1}{N} \sum_{n=1}^{N} u_{i,m,n} \right) \right) \tag{1}$$

subject to:

(a) Water quality constraints:

$$LO \le y_{i,n} \le UP \tag{2}$$

(b) State of water quality transition equations:

$$
\begin{aligned}
&\text{Tributary segments:} && y_{i,n} = \qquad x_{i,n} - \sum_{m=1}^{M} u_{i,m,n} \\
&\text{Downstream segments:} && y_{i,n} = \sum_{\substack{upstream\\ seg.\,of\,i}} y_{i,n} + x_{i,n} - \sum_{m=1}^{M} u_{i,m,n} \quad \forall \; i,n
\end{aligned}
\tag{3}
$$

(c) Technology capacity constraints:

$$
u_{i,m,n} \le c_m b_{i,m}, \quad \forall \;\; n \tag{4}
$$

(d) Constraints on choice variables:

$$
\begin{aligned}
&u_{i,m,n} \;\; \ge 0 \\
&b_{i,m} \;\;\; = 0 \;\; or \;\; 1 \qquad \forall \;\; i, m, n
\end{aligned}
\tag{5}
$$

(e) Technology selection constraints:

$$
\sum_{m} b_{i,m} \le 1 \qquad \forall \;\; i \tag{6}
$$

where,

$x_{i,n} \equiv y_{i,n}^{0}$ for tributary segments

$x_{i,n} \equiv y_{i,n}^{0} - \sum_{\substack{upstream\\ seg.\,of\,i}} y_{i,n}^{0}$ for downstream segments

i is the index for stream segments or reaches.

m is the index for treatment technologies.

n is the number of observations drawn to re-generate the statistical distributions of pollution loadings (y^{0}_{i}).

$u_{i,m,n}$ represent the choice or decision variables. There are *n* such variables for each stream segment.

$v_{i,m}$ represent the variable costs or the per unit cost of treatment with technology *m* for segment *i*.

$f_{i,m}$ represent the fixed costs or set-up costs for technology *m* for segment *i*.

$y_{i,n}^{0}$ represent the initial states of water quality for segment *i*. The distribution and parameters of this variable are determined from existing data. The optimization model draws random observations following those parameters to re-generate the distributions.

$y_{i,n}$ represent the post-treatment states of water quality for stream segment *i* resulting from a positive level of treatment. The levels of treatment must be chosen in such a way such that the post-treatment water quality remains within the lower (*LO*) and upper (*UP*) bounds of the mandatory standards.

$b_{i,m}$ is a binary auxiliary choice variable for stream segment *i*. It assumes the value 1 when treatment is chosen by technology *m,* and 0 otherwise.

$x_{i,n}$ represent residual or exogenous pollution drainage to segment *i* from respective sub-watersheds.

c_m represent the capacity of plants of treatment technology *m*.

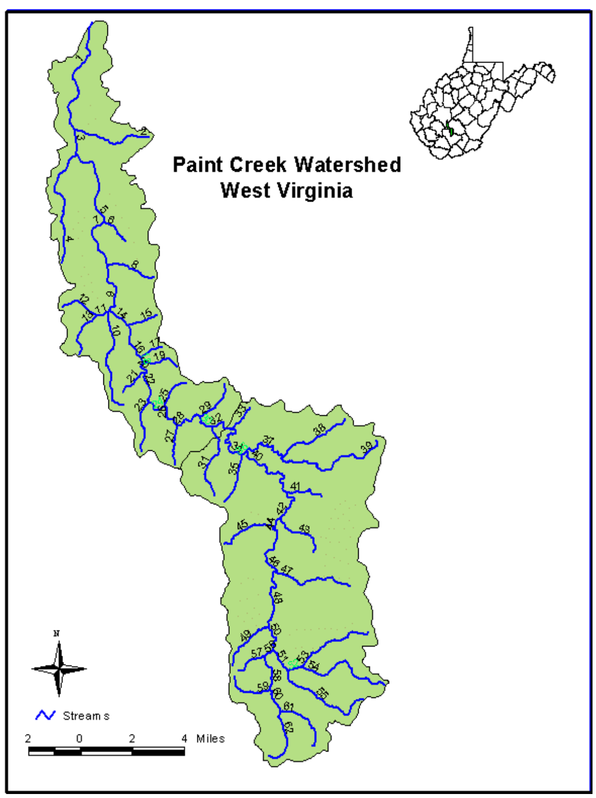
The objective function in this model minimizes total expected costs which is the sum of fixed costs and average variable costs. The fixed costs are added to the total only when $b_{i,m} = 1$, i.e., when treatment is required. The levels of treatment are determined in such a way that water quality standards (2), mass-balance conditions (3), and technology capacity constraints (4) are maintained. An optional constraint (6) is also defined to limit the number of technologies to one per segment. It may or may not be included in the model depending on the preference of the policy makers and the specifics of the problem to be addressed.

Any number of observations *N* can be drawn to re-generate the distributions of the stochastic variables depending on the level of accuracy required. However, since each observation also increases the number of constraints in the model, there is a direct trade-off between model size and statistical accuracy. For this general model, the number of constraints can be derived from the expression $[I \times N\ (3 + M) + I]$ and the number of variables from $[I \times N\ (1 + M) + I \times M]$. The primary difference of this stochastic model over other stochastic approaches such as chance-constrained programming and first-order uncertainty analysis is that unlike the chance-constrained models where the constraints are satisfied with a predetermined confidence levels, all constraints are satisfied in this approach with 100 percent certainty. Unlike the first-order uncertainty analysis, this approach does not depend on the first two moments only. The level of significance is controlled by the process that draws the observations to be included in the model. Any level of probability can be specified by the cut-off point selected in this simulation process.

Application – AMD Treatment in the Paint Creek Watershed

To demonstrate the application of the methodology, the model described by equations (1) through (6) is adapted to estimate the pH TMDL implementation costs for the Paint Creek watershed located in south-central West Virginia. Total drainage area of this watershed is about 123 square miles. The stream network is composed of 62 segments, 32 headwater or tributaries and 30 downstream segments, which serve to divide the watershed into 62 catchments or sub-watersheds.

Paint Creek, a tributary of the Kanawha River, flows north through 24 small communities with a combined population of about 7,200. Over the past 90 years both surface and deep coal mining activities have taken place in this watershed, but very little attention was paid to environmental degradation resulting from mining activities until the passage of the West Virginia Surface Coal Mining and Reclamation Act (WVSCMRA) and the Surface Mining Control and Reclamation Act (SMCRA) in 1977.



After coal extraction, mine openings and boreholes were abandoned allowing surface water to seep into deep mines and react with sulfur and metal ions to form acidic solutions. These acidic solutions flow out of the mine to the adjacent streams and tributaries. The West Virginia Department of Environmental Protection (WVDEP) and the Paint Creek Watershed Associations conducted water sampling at locations in both the mainstream and tributary segments. The water in many locations was highly acidic and far exceeded the West Virginia water quality standards which require waters to be between pH 6.0 and 9.0.

Data Sources

Data for the empirical model of the Paint Creek watershed were obtained from two major sources. Daily estimates of water flow and net acidity for all 62 stream segments for a five year period (1992-96) were generated by the *Total Acidic Mine Drainage Loadings (TAMDL)* model. *TAMDL* is a computer simulation model developed by Stiles (2002) at the West Virginia Water Resources Institute, West Virginia University to provide the analytical capabilities necessary to model in-stream concentrations and reaction of the various constituents of acid mine drainage (AMD). The output of the *TAMDL* model provided estimates of flow level and acid loadings in units of $CaCO_3$ equivalent per year. *TAMDL* was applied as part of the development of the TMDL allocations for the Paint Creek Watershed (USEPA, 2001b).

Detailed information on plant sizes and related fixed costs of operation for four alkaline treatment technologies – soda ash (Na_2CO_3), caustic soda ($NaOH$), ammonia (NH_3), and hydrated lime ($Ca(OH)_2$) – as well as per unit chemical reagent costs were obtained from various studies conducted by Fletcher et al. (1991) and Phipps et al.

(1996). Soda ash based technologies can be applied to treat smaller amounts of acidity with a plant capacity of 10 metric tons of $CaCO_3$ equivalent acid per year. The other three technologies can be applied to a wide range of flow-acidity conditions but may require bigger capacity plants for high-flow-high-acidity waters. Treatment capacities of two different plant sizes for caustic soda and ammonia and four different plant sizes for hydrated lime were used. For caustic soda and ammonia, the derived capacities were 10 and 4,975 metric tons of $CaCO_3$ equivalent per year, and for hydrated lime, the derived capacities were 10, 199, 249, and 4,975 metric tons of $CaCO_3$ equivalent acid per year respectively. The model treated the various combinations as separate technologies – a total of nine plant size, chemical technology combinations.

The Specific Model

The specific model for the Paint Creek watershed is thus written with 62 stream segments and 9 technologies. The objective function takes the form:

$$\text{Minimize} \quad \text{E(cost)} = \underset{\{u_{i,m}\}}{Min} \sum_{i=1}^{62} \sum_{m=1}^{9} \left(f_{i,m} b_{i,m} + v_{i,m} \left(\frac{1}{N} \sum_{n=1}^{N} u_{i,m,n} \right) mwt_m \right) \tag{7}$$

The mwt_m term represents the molecular weight factor of the chemical reagent used in technology m. It is defined as the product of the ratio of the molecular weight of a reagent to the molecular weight of $CaCO_3$ and the number of units of that reagent is needed to neutralize one unit of $CaCO_3$ equivalent acid load. Some chemicals such as ammonia and sodium hydroxide require two units to neutralize one unit of $CaCO_3$ equivalent acid. The product of the average treatment levels $\left(\frac{1}{N} \sum_{n=1}^{N} u_{i,m,n} \right)$ and molecular weight factor mwt_m gives the amount (in metric tons/year) of reagent m required for treatment. This amount is then multiplied by the \$/metric ton costs of reagent m, $v_{i,m}$, to derive the total average variable costs in \$/year. The water quality constraints are written as:

(a') Water quality constraints:

$$\begin{aligned}&\text{Upper bound: } y_{i,n} \leq w_{i,n} \times s6 \times k\\&\text{Lower bound: } y_{i,n} \geq w_{i,n} \times s9 \times k\end{aligned} \tag{8}$$

where, s6 and s9 represent the mg/L equivalent net acidity corresponding to pH 6 and 9 respectively. Since water flows ($w_{i,n}$) are measured in gallons per minute, the right-hand-sides of these two equations give the allowable upper and lower bounds of acid loadings corresponding to the West Virginia water quality standards expressed in metric tons of $CaCO_3$ equivalent acid load per year.

The water quality transition equations following the mass-balance conditions are expressed as,

(b') State of water quality transition equations:

$$\begin{aligned}&\text{Tributary segments: } y_{i,n} = x_{i,n} - \sum_{m=1}^{9} u_{i,m,n}\\&\text{Downstream segments: } y_{i,n} = \sum_{\substack{upstream\\ seg.\,of\,i}} y_{i,n} + x_{i,n} - \sum_{m=1}^{9} u_{i,m,n}\end{aligned} \tag{9}$$

The only modification in these two sets of equations is that the total number of treatment technologies m is now defined. The technology capacity constraints remain the same as they were in the generic model with i and m explicitly defined.

(c') Technology capacity constraints:

$$u_{i,m,n} \leq c_m b_{i,m}, \ \forall\ n \tag{10}$$

The constraints on the choice variables also remain the same as in the generic model.

(d’) Constraints on choice variables:

$$\begin{aligned} &u_{i,m,n} \geq 0 \\ &b_{i,m} = 0,\ or\ \ 1 \end{aligned} \tag{11}$$

Finally, the technology selection constraints are modified to indicate the nine technologies included in the Paint Creek model.

(e’) Technology selection constraints:

$$\sum_{m=1}^{9} b_{i,m} \leq 1,\ \forall\ \ i \tag{12}$$

Assumptions

In addition to the mass-balance conditions of the generic model, three more assumptions are made for the specific Paint Creek model due to unavailability of appropriate information. These are:

(1) Water flow and acid loadings are independent. In reality, there is a negative covariance between these two variables. The implication of this assumption is that the estimates of acid loadings and treatment levels will be higher. As a result, treatment costs are overestimated in this study.

(2) No variations in the set-up costs of treatment technologies across different sub-watersheds. In reality, these costs are expected to vary because of the topography, accessibility, unavailability of electricity, etc.

(3) Per unit treatment costs do not change with the level of treatment for the same chemical but different capacity plants. However, they do vary for different chemical technologies.

Distributions of Water Flow and Net Acidity

The five-year daily data on water flow and net acidity for all 62 stream segments of the Paint Creek watershed obtained from the *TAMDL* model were tested with the distribution fitting software *BestFit* (Palisade Corporation, 2000) to determine the appropriate distributions and the related parameter estimates. It was observed that water flow follows the lognormal distribution and net acidity follows the triangular distribution for almost all segments. Some minor adjustments were made for those segments where lognormal and triangular were not a perfect fit. Parameters of these distributions were noted and used to re-generate these distributions through random draws in the optimization model.

Two transformation functions linking a standard normal variable to the lognormal parameters and a standard uniform variable to the triangular parameters were used in the optimization programs to transform the normal and uniform variables directly available in *GAMS* (Brook et al., 1998) as appropriate.

The triangular distribution is bounded by the minimum and maximum values while the lognormal distribution is unbounded. The characteristic fat tail of the lognormal probability density function (pdf) is asymptotic to the horizontal axis. The implication is that the probability of obtaining an extremely large observation is never zero; random observations drawn from the lognormal distribution will be arbitrarily large with some positive probability. Acid loadings corresponding to these observations will also be large and may go well beyond the treatment capacity of all feasible plants resulting in infeasible model solutions. Even when the solution is feasible, the optimal solution will include larger capacity treatment plants at a very high fixed cost and may significantly overstate any observed or expected outcome.

To avoid this problem, an upper limit or treatment up to a selective percentile of the distribution was used in the model, not the complete distribution. A large number of observations (50,000) for the acid loadings for all 62 stream segments were drawn to serve as the empirical distribution. These draws were then sorted in ascending order and the 90th, 95th, 97th, 99th, and 99.9th percentile values noted. During the optimization process, if any random draw resulted in a value greater than the appropriate percentile values for a given run, they were censored appropriately. The model was run with 700 sample observations for each of the percentile levels of treatment noted above and treatment levels, fixed, and variable costs compared.

Methodology

The MIP model for the Paint Creek watershed was estimated using the *CPlex* solver available with the *GAMS* software. The lognormal and triangular parameters obtained from the *BestFit* software were used in the *GAMS* program and transformation functions were used to link these parameters with draws from standard normal and standard uniform variables to re-generate the distributions of lognormal water flow and triangular net acidity. The simulated flow and acidity data were then used to calculate the acid loadings included in the optimization model. All stream segments were assigned the same randomly drawn value in a particular draw to reflect the high spatial autocorrelation between flows and loadings at a specified point in time. The implication of this drawing process is that any change in the upstream loadings will affect the downstream loadings proportionately and is in accordance with the mass balance approach used in the linear approximation. During the optimization process, a suitable number of sample observations for lognormally distributed water flow and triangularly distributed net acidity were drawn and corresponding acid loadings calculated and checked against those percentile values. Loadings that exhibit values greater than a specific percentile value were replaced by that percentile value. The *GAMS/Cplex* solvers used dual simplex and branch-and-bound algorithms.

Results

Increasing the percentile values implies usage of more area from the positively skewed tail of the lognormal distribution. This increases the probability of encountering more extreme observations in the optimization process. For the present problem, these more extreme values simply mean higher levels and costs of treatment. If a larger plant is required to treat the higher load, this may require installation of higher capacity treatment plants as well. This issue is investigated for a fixed sample size of 700 observations and for variable levels of treatment. The results are presented in Table 1.

Summary results in Table 1 suggest that total expected costs (TEC) of treatment increase with increases in the percentile of loads fully treated. The increase in the cost is primarily due to the higher amount of acid treatment which sometimes requires higher capacity treatment plants. Smaller caustic soda plants were sufficient to meet the treatment requirements for the 90th percentile treatment. When the required level of treatment increases from the 90th to the 95th percentile, smaller caustic soda plant originally selected for stream segment 4 is no longer sufficient. For treating the 97th percentile treatment, segments 4 and 33 both require larger caustic soda plants. For even higher 99th percentile treatment level, stream segments 4, 33, 43 and a new segment 13 which do not require any treatment previously for lower bounds, also need the larger caustic soda plants. This increased capacity simply translates to higher fixed costs.

With 700 sample observations, the activity matrix had 520,862 rows and 434,558 columns with 1,736,417 non-zero elements. The proportion of non-zero elements was 7.67×10^{-6}. The *CPlex* solver used 153,969 iterations to achieve the optimum solution and required 1.7 GB virtual memory and 21 minutes CPU time with a P-III 550.

Table 1: Effects of Different Percentile Treatment on Total Expected Costs

Results for sample size = 700

Segments to be treated	Least-cost method of treatment	Average acid load to be treated (mt/yr)	Average reagent requirement (mt/yr)	Annualized Fixed cost (F) ($/yr)	Average variable cost (AVC) ($/yr)	Total Expected cost, TEC = (F + AVC) ($/yr)	Coefficient of variation for acid load treated
90th percentile treatment							
4	C. Soda-1	0.27	0.22	7,045.00	104.80	7,149.80	3.44
10	Ammonia-2	210.68	71.63	10,050.00	23,638.03	33,688.03	1.23
12	Ammonia-2	174.62	59.37	10,050.00	19,592.32	29,642.32	1.50
19	Ammonia-2	13.48	4.58	10,050.00	1,511.94	11,561.94	1.38
21	Ammonia-2	19.42	6.60	10,050.00	2,178.78	12,228.78	1.63
25	Ammonia-2	43.51	14.79	10,050.00	4,881.55	14,931.55	1.13
33	C. Soda-1	1.09	0.87	7,045.00	422.80	7,467.80	1.10
43	C. Soda-1	0.03	0.02	7,045.00	11.61	7,056.61	5.67
57	C. Soda-1	0.003	0.002	7,045.00	1.21	7,046.21	6.42
Total for all segments		463.09		78,430.00	52,343.04	130,773.04	
95th percentile treatment							
4	C. Soda-2	0.66	0.53	7,498.00	257.17	7,755.17	3.39
10	Ammonia-2	260.97	88.73	10,050.00	29,280.83	39,330.83	1.51
12	Ammonia-2	231.01	78.54	10,050.00	25,919.22	35,969.22	1.81
19	Ammonia-2	23.65	8.04	10,050.00	2,653.57	12,703.57	3.12
21	Ammonia-2	29.40	9.99	10,050.00	3,298.24	13,348.24	2.22
25	Ammonia-2	57.37	19.51	10,050.00	6,437.33	16,487.33	1.49
33	C. Soda-1	1.42	1.14	7,045.00	549.81	7,594.81	1.23
43	C. Soda-1	0.09	0.07	7,045.00	33.95	7,078.95	4.78
57	C. Soda-1	0.01	0.01	7,045.00	3.41	7,048.41	6.80
Total for all segments		604.58		78,883.00	68,433.53	147,316.53	
97th percentile treatment							
4	C. Soda-2	1.01	0.81	7,498.00	390.78	7,888.78	3.64
10	Ammonia-2	289.83	98.54	10,050.00	32,518.79	42,568.79	1.70
12	Ammonia-2	264.03	89.77	10,050.00	29,624.00	39,674.00	2.05
19	Ammonia-2	28.39	9.65	10,050.00	3,185.24	13,235.24	3.71
21	Ammonia-2	34.58	11.76	10,050.00	3,879.55	13,929.55	2.33
25	Ammonia-2	74.43	25.31	10,050.00	8,351.51	18,401.51	2.10
33	C. Soda-2	1.60	1.28	7,498.00	618.03	8,116.03	1.33
43	C. Soda-1	0.15	0.12	7,045.00	58.94	7,103.94	5.00
57	C. Soda-1	0.01	0.01	7,045.00	5.40	7,050.40	10.00
Total for all segments		694.03		79,336.00	78,632.25	157,968.25	
99th percentile treatment							
4	C. Soda-2	1.66	1.33	7,498.00	642.88	8,140.88	4.15
10	Ammonia-2	328.93	111.84	10,050.00	36,905.95	46,955.95	2.07
12	Ammonia-2	308.92	105.03	10,050.00	34,660.37	44,710.37	2.47
13	C. Soda-2	4.51	3.61	7,498.00	1,745.18	9,243.18	10.16
19	Ammonia-2	45.75	15.55	10,050.00	5,132.80	15,182.80	6.17
21	Ammonia-2	65.5	22.27	10,050.00	7,348.57	17,398.57	4.58
25	Ammonia-2	84.08	28.59	10,050.00	9,433.83	19,483.83	2.42
33	C. Soda-2	1.84	1.47	7,498.00	713.27	8,211.27	1.55
43	C. Soda-2	0.27	0.22	7,498.00	105.13	7,603.13	5.30
57	C. Soda-1	0.02	0.02	7,045.00	8.25	7,053.25	7.00
Total for all segments		841.47		87,287.00	96,696.23	183,983.23	

mt/yr = metric tons of $CaCO_3$ eq per year
Averages were taken over the sample size
C. Soda-1 = Smaller caustic soda plant for low-flow-acidity waters
C. Soda-2 = Larger caustic soda plant for moderate to high flow-acidity waters
Ammonia-2 = Larger ammonia plant for moderate to high flow-acidity waters
Fixed cost includes all costs other than chemical cost
Annualized fixed cost was calculated assuming a 20-year plant life and a 6% discount rate

Margin of Safety (MOS)

The TMDL guidelines suggest an *ad hoc* adjustment to the end-points of allowable loads in determining MOS inclusive load allocations for point and non-point sources. This approach sidesteps the requirements of examining the actual statistical distributions of pollutant loadings. Implementation of such TMDLs requires building larger capacity treatment plants at higher costs. If the true distributions of loadings were known, allocations would have been lower, requiring lower implementation costs. The different costs of these two scenarios would then be interpreted as the savings due to the knowledge of the true MOS.

Since the distributions of polluting variables are known in this study, arbitrary adjustments to the end-points of allowable loads are not necessary to get an estimate of savings due to the knowledge of MOS. Rather, it is possible to determine the exact amount of treatment to be carried out or the level of plant capacity to be built to achieve a target level of assurance. This approach is followed in the present study to estimate the savings due to the knowledge of MOS corresponding to different levels of assurance. Since the 100th percentile treatment of acid load is empirically impossible in the present approach due to the presence of the asymptotic tail, the maximum attainable level of safety was assumed to be with the 99.9th percentile treatment. Costs associated with this level of assurance were compared with that of a more pragmatic and attainable goal of the 95th to 99th percentile treatment. The differential costs provide the estimates of savings for the knowledge of MOS. The results are presented in Figure 1.

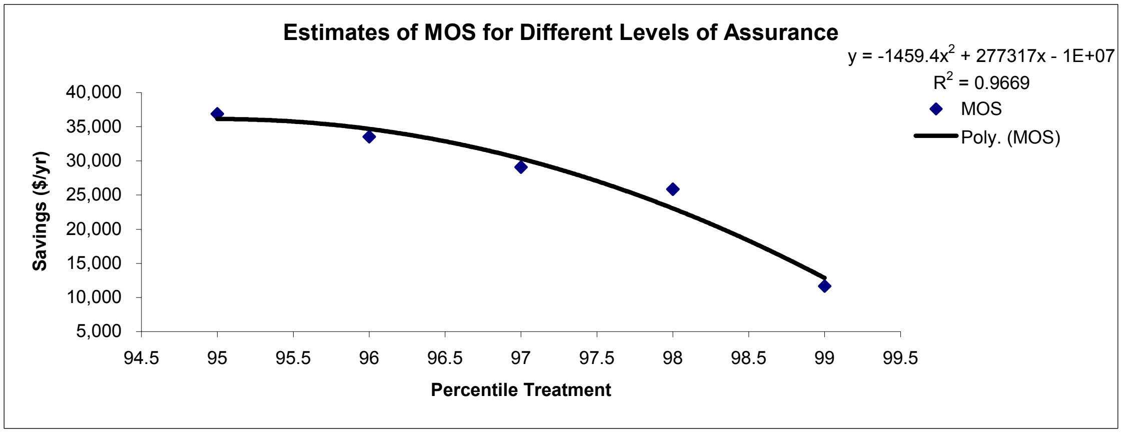


Figure 1: Estimates of Margin of Safety for Different Levels of Assurance

The vertical axis of this graph represents the difference in total expected treatment costs of the 95th to 99th percentile treatment levels from that of the 99.9th percentile treatment. They can be interpreted as the savings in treatment costs for a guaranteed 95 to 99 percent assurance. The graph indicates that savings decrease at an increasing rate with the levels of assurance. Treatment costs are 7 percent lower when 99 percent assurance is desired. If the required level of assurance is lowered to 95 percent, then 21 percent lower treatment cost could be achieved.

Pollution Trading

The watershed approach of the TMDL process and the spatial linkage of streams allow pollution trading when set-up costs for treatment plants vary across sub-watersheds. The spatial network of streams allows treatment of a downstream segment through addition of alkalinity in that stream or anywhere upstream. The implication is that low-cost sources upstream can negotiate with high-cost sources downstream to gain from trade through treatment by the low-cost sources. This issue is illustrated with the help of a deterministic version of the model estimated with constant average values of water flow and net acidity data and with reduced fixed cost for a specific segment. The results are presented in Table 2.

Table 2: Potentials for Pollution Trading

Segments to be treated	Least-cost method of treatment	Optimal acid load to be treated (mt/yr)	Chemical reagent requirement (mt/yr)	Annualized Fixed cost (FC) ($/yr)	Variable cost (VC) ($/yr)	Total Cost TC=FC+VC ($/yr)
Deterministic Model Results						
10	Ammonia-2	169.05	57.48	10,050.00	18,967.52	29,017.52
11	Ammonia-2	104.05	35.38	10,050.00	11,674.85	21,724.85
19	Ammonia-2	21.28	7.23	10,050.00	2,387.19	12,437.19
25	Ammonia-2	39.21	13.33	10,050.00	4,399.74	14,449.74
33	C. Soda-1	1.90	1.52	7,045.00	735.55	7,780.55
Total for all segments		335.49		47,245.00	38,161.31	85,409.85
Results When Fixed Costs of Technology for Segment 12 were Reduced by $1000						
10	Ammonia-2	169.05	57.48	10,050.00	18,967.52	29,017.52
12	Ammonia-2	104.05	35.38	9,050.00	11,674.85	20,724.85
19	Ammonia-2	21.28	7.23	10,050.00	2,387.19	12,437.19
25	Ammonia-2	39.21	13.33	10,050.00	4,399.74	14,449.74
33	C. Soda-1	1.90	1.52	7,045.00	735.55	7,780.55
Total for all segments		335.49		46,245.00	38,164.85	84,409.85

mt/yr = metric tons of CaCO3 eq per year
C. Soda-1 = Smaller caustic soda plant for low flow-low acidity waters
Ammonia-2 = Larger ammonia plant for moderate to high flow-acidity waters
Fixed cost includes all costs other than chemical cost
Annualized fixed cost was calculated assuming a 20-year plant life and a 6% discount rate

The upper panel of this table shows that the deterministic model has selected five stream segments – 10, 11, 19, 25, and 33 – in the optimal solution. Among these five segments, only 11 is a downstream segment and others are tributary segments. For tributaries, the model has no choice but to treat them individually. For downstream segment 11, however, the model can neutralize acidity problems through the injection of excess alkalinity into its upstream segments 12 or 13 if costs are lower. The lower panel shows the results when the model was run again with the fixed installation cost for treatment technology for segment 12 reduced by $1000. The optimal solution in this case included the low-cost segment 12 instead of the previously selected segment 11.

The implication of this exercise is that if the sources in sub-watershed 11 have higher costs for treatment, they can negotiate with the lower cost sources in sub-watersheds 12 or 13 to come up with a cheaper cost alternative strategy. Sources in sub-watershed 11 would be willing to offer any price lower than $21,724.85 for this clean-up activity while sources in sub-watershed 12 or 13 would be willing to take any price above $20,724.85. Both parties will be benefited from this trade and a Pareto optimal improvement in the solution will be achieved.

Estimates of Inter-temporal Variations

The effect of inter-temporal variations was investigated by comparing the results of the stochastic model with that of the deterministic model. The difference in the total minimized costs indicates the extent of underestimation in treatment costs if variability in stream conditions is ignored.

Table 3: Estimates of Treatment Costs Due to Inter-temporal Variations

Models	Total cost ($/yr)
Stochastic (97th percentile treatment)	157,968.25
Deterministic	85,409.85
Under-estimate with deterministic model	72,558.40

Table 3 shows that if the variability in stream conditions is not accounted for in the model, treatment costs are underestimated significantly. The deterministic model, which was estimated with constant average flow and acidity assumptions, underestimated treatment cost by about 45 percent relative to the 97th percentile stochastic model. The implications of neglecting the inter-temporal variations are that the treatment plants would be under-capacity and actual treatment costs would be grossly underestimated.

Alternatively, the treatment levels would be far from sufficient a significant proportion of the time.

Conclusions

In this paper, a stochastic mixed-integer programming methodology is presented to address the inter-temporal variations in pollution loadings in the stream network of a spatially integrated watershed. Traditional programming approaches are unsatisfactory for the assumptions on which they are based or are inadequate when distributions are not normal. The proposed methodology makes no *a priori* assumptions, rather estimates distribution parameters from simulated data to use in the optimization process. The methodology is applied to estimate pH TMDL implementation costs for the Paint Creek watershed in West Virginia. The empirical model provided information on which stream segments should be treated, the method of treatment, the levels of treatment for which investments need to be made, and the estimated cost. The model also indicates the trade-off between treatment plant capacities and the level of assurance or margin of safety. The approach allows a clear calculation of the cost of increased margins of safety and should provide input to stimulate discussion of potential trade-offs possible within a watershed framework.

A deterministic version of the model is also estimated with average levels of water flow and net acidity for the Paint Creek streams. The optimal solution included four tributary segments and one downstream segment for treatment. These results are compared with that for another run of the deterministic model which included a reduced fixed set-up costs for a specific upstream segment to demonstrate the potentials for pollution trading. Results show that when abatement costs differ among sources, it is possible to gain from trade through treatment by lower cost sources.

A comparison of stochastic and deterministic model results indicates that when inter-temporal variability in stream conditions is ignored, the treatment cost is underestimated significantly; the difference between the deterministic and the 97th percentile treatment with the stochastic model is about 45 percent.

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