# L-Shaped BONUS Algorithm with Application to Water Pollutant Trading

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Applications of optimization in the field of process systems engineering often involve dealing with nonlinearity and uncertainty, necessitating the solution of stochastic nonlinear programming (SNLP) problems. However, the existing algorithms to solve such problems suffer from various limitations. The L-shaped BONUS algorithm, which is an integration of the BONUS (Better Optimization of Nonlinear Uncertain Systems) algorithm and the sampling-based L-shaped method, has been recently proposed to overcome some of these problems. It is shown to have desirable computational properties. This work further investigates the properties of the algorithm by applying it to the environmental problem of pollutant (nutrient) trading in the Christina River Basin. With environmental concerns being heightened, pollution abatement-related decisions are important for industry, making efficient solution techniques invaluable. The results confirm the computational efficiency of the L-shaped BONUS algorithm. Simultaneously, interesting aspects of the environmental trading problem are also explored, pointing toward the scope of implementing stochastic programming techniques for better decision making in the field of industrial ecology.



## 1. Introduction

Stochastic nonlinear programming (SNLP) problems represent an important class of optimization problems because of their omnipresence in real-life situations. Many systems in nature are inherently nonlinear, necessitating nonlinear models for their representation and consequently, nonlinear programming methods for optimization. Another important factor for consideration is uncertainty. Very rarely are the system details accurately known. Quite often, the parameters and variables are known only in terms of their ranges or, in some cases, in terms of their probability distributions. In such cases, optimization necessitates the use of stochastic programming methods.

The field of process systems engineering is replete with applications of stochastic programming, many of which are nonlinear. Numerous well-known tasks in this field, such as project planning and scheduling, chemical synthesis, process design and optimization, and some new fields (such as computer-aided molecular design), use stochastic programming. An extensive review of various stochastic programming methods and their applications in process engineering field is presented in the work of Diwekar[1] and Sahinidis.[2] Some recent applications include enterprise-wide process network,[3] planning and scheduling related tasks,[4,5] and environment-related applications.[6−8] Many of these problems are nonlinear, complicating the solution to the problem.

However, despite the relative importance of such problems, comparatively few solution methodologies have been determined to be successful over the entire domain of problems in this class. Computational requirement is the major hurdle for many algorithms. Among the various solution methodologies proposed, sampling-based approaches have become particularly popular because they are able to reduce the computational requirements to a certain extent. However, these approaches also become computationally inefficient if the problem to be solved is nonlinear and/or high-dimensional. To alleviate the computational hurdles, a new algorithm, the L-shaped BONUS algorithm, has been recently proposed by Shastri and Diwekar.[9] It has been shown to offer considerable advantages over the traditional sampling based approach through its application to different problems.[9,10] This article intends to further investigate the properties of the L-shaped BONUS algorithm by applying it to an interesting environmental problem.

With environmental regulations becoming increasingly stringent, waste management decisions are becoming important for industrial sustainability. Consequently, innovative ideas for waste management to reduce the financial burden are being sought. Pollutant credit trading is one such approach.[11] Pollutant trading has been introduced with the desire to achieve an economic approach for optimal resource management (i.e., to achieve environmental targets at a lower overall cost). A recent agreement between the United States Environmental Protection Agency (USEPA) and the United Stated Department of Agriculture (USDA) to promote market-based approaches (trading) to improve water quality is testimony to the heightened interest in the trading approach. However, industry-level decision making in this integrated setup is difficult, particularly in the presence of uncertainty. Therefore, this work applies the L-shaped BONUS algorithm to the pollutant trading problem to optimize such decisions. The trading problem presented in this paper focuses on the its application to water pollutants that affect aquatic systems such as ponds, lakes, or rivers.

Thus, the purpose of this article is two-fold. The work investigates the properties of the L-shaped BONUS algorithm using a new problem, and it also attempts to explore the various tradeoffs and dynamics associated with the problem of pollutant trading. The remainder of the article is organized as follows. The next section discusses the L-shaped BONUS algorithm; it first presents an overview of the current SNLP solution methods and then discusses the L-shaped BONUS algorithm. Section 3 explains optimization problem formulation for nutrient trading. The Christina River Basic nutrient management problem is initially presented, and the optimization model for the case is then formulated. Section 4 presents the results for the pollutant trading problem and also presents a summary of the results for other problems solved using the proposed algorithm. The paper ends with concluding remarks in section 5.

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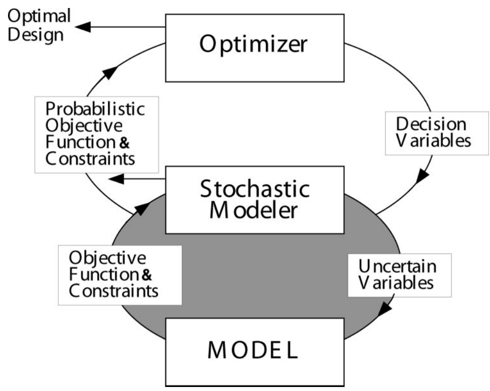


**Figure 1.** Sampling-based optimization algorithm structure.

## 2. L-Shaped BONUS Algorithm

**2.1. SNLP Problems: Overview.** A general stochastic nonlinear programming problem can be represented as follows:

$$\text{Optimize } J = P_1(f(\theta, x, u)) \tag{1}$$

such that

$$P_2(g_1(\theta, x, u)) = 0 \tag{2}$$

$$P_3(g_2(\theta, x, u) \leq 0) \geq \alpha \tag{3}$$

where, $\theta$ is the set of decision variables, $x$ the set of system parameters, and $u$ the set of uncertain variables. $P_1$, $P_2$, and $P_3$ are probabilistic measures such as expected value or variance. Uncertainty may affect the objective function and/or any of the constraints to make it a stochastic programming problem.

Over the years, much research has been focused on devising strategies to solve the SNLP problems. One type of solution method—the chance constraint programming method[12]—converts these problems to deterministic equivalents. A second type of solution method is aimed at extending the deterministic nonlinear programming methods to include uncertainty.[13−15] For optimization problems that can be decomposed into two or multiple stages, decomposition-based stochastic programming methods, such as the L-shaped method, are developed.[16] These decomposition-based methods require convexity of the problem and/or a dual-block angular structure. The stochastic quasi-gradient (SQG) methods are less specialized than the other algorithms, but they are useful for solving problems that have complex objective functions and constraints.[17] SQG methods represent one of the first computational developments in stochastic programming. While decomposition methods and SQG methods provide improvements based on optimization algorithms, the sampling-based approaches improve the accuracy and efficiency of the uncertainty analysis part of the stochastic programming algorithms. The following subsection discusses the sampling-based L-shaped method.

**2.2. Sampling-Based L-Shaped Method.** Sampling-based approaches have often been used, because of their computational advantages. The objective is to model the complete uncertain parameter space as closely as possible using a sufficient number of samples. The overall algorithm structure is represented in Figure 1. The structure of the algorithm is similar to that for a deterministic problem, apart from the fact that the deterministic model is replaced by a stochastic model with the sampling loop representing the discretized uncertainty space. The goal in stochastic programming is to improve the probabilistic objective function value with each iteration. The calculation of these terms requires simulation of the stochastic modeler at each iteration. In the traditional sampling-based methods, this is achieved by model simulations for a given number of samples, and the subsequent computation of the probabilistic function (such as the expected value of the objective function).

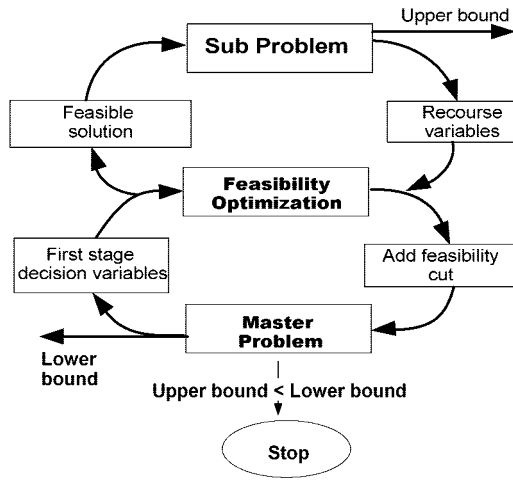


**Figure 2.** L-shaped algorithm structure.

The L-shaped method is a scenario-based method.[18,19] However, the number of scenarios increases exponentially as the number of uncertain variables increases. Monte Carlo sampling avoids this problem and, hence, Monte Carlo sampling-based approximations have been incorporated in the L-shaped method. The key feature is the use of statistical estimates to obtain confidence intervals on the results. The sampling-based L-shaped method is schematically shown in Figure 2. The given problem is first decomposed into two or multiple stages. The first-stage (master) problem uses linear approximation of the second-stage nonlinear recourse function. The first-stage decisions are passed to the second-stage problem (subproblem), where the expected value of the nonlinear recourse function is computed exactly, using the given samples. The second-stage problem solution is used to generate the feasibility and optimality cuts for the master problem for better approximation. The procedure is continued until the statistical termination criteria are satisfied.

It can be observed that the second-stage problem must be solved for every sample at every iteration of the algorithm. If the problem solution is dependent on the value of a model variable, then the model must be simulated for each sample in an iteration and at each such iteration. This is a severe limitation of this approach. When the model is high dimensional and/or nonlinear, the simulation requirement can seriously impede the speed of the algorithm.

**2.3. Better Optimization of Nonlinear Uncertain Systems (BONUS).** Sampling-based stochastic programming approaches suffer from the drawback of repeated model simulations at the stochastic modeler stage. To overcome this problem, Sahin and Diwekar[20] proposed a new algorithm, called BONUS (Better Optimization of Nonlinear Uncertain Systems). The algorithm structure, which is quite similar to the general sampling based algorithm, is schematically represented in Figure 3. It differs from the standard sampling-based algorithms in regard to the uncertainty propagation step, where it incorporates the reweighting approach.

The reweighting scheme, which is based on various schemes proposed by Hesterberg,[21] is used to estimate the probabilistic function value of the output distribution without evaluating the model for the input distribution, provided the output for some other input distribution is known using rigorous simulations. The reweighting scheme, as used in an optimization algorithm,

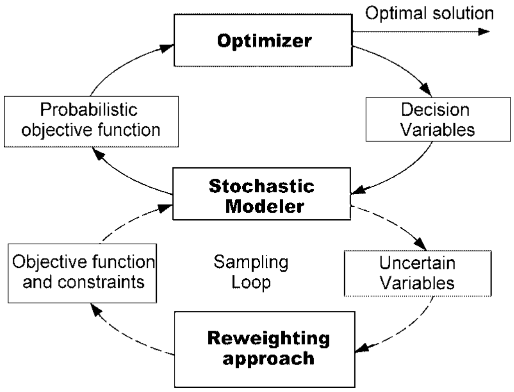


**Figure 3.** BONUS algorithm.

is illustrated in Figure 4. Suppose $X$ represents the uncertain variable in the stochastic programming problem, and $Q(X)$ is the output of the stochastic modeler. For the first optimization iteration, the base case samples $X_i^*$ with uniform distribution ($\hat{f}(x)$) are drawn, and the model is simulated for each sample to get the complete model output distribution $Q(X_i^*)$. During the subsequent iterations, when the optimizer requires new estimates of the probabilistic objective function for a new sample set, new samples $X_i$ of the required distribution ($f(x)$) are drawn. Having known the model response $Q(X_i^*)$ for the base sample set $X_i^*$ from the distribution $\hat{f}(x)$, a reweighting-based relationship can be used to compute the expected value of the model response $Q(X_i)$ for the new sample set $X_i$ from the distribution $f(x)$. Therefore, the expected value of the stochastic model response $Q(X_i)$ for the new sample set $X_i$ is given as

$$E_f[Q(X_i)] = \sum_{j=1}^{N_{\mathrm{samp}}} w(j) Q(X_j^*) \tag{4}$$

where $w(j)$ are the weights, computed using the two density functions, as

$$w(j) = \frac{\dfrac{f(X_j)}{\hat{f}(X_j^*)}}{\sum_{i=1}^{N_{\mathrm{samp}}} \dfrac{f(X_i)}{\hat{f}(X_i^*)}} \tag{5}$$

Here, $N_{\mathrm{samp}}$ is the sample size. The determination of the probability distribution from the sample sets is performed using Gaussian Kernel Density Estimation,[22] which is a nonparametric density estimation technique. An exhaustive description of the reweighting scheme can be found in the work of Hesterberg[21] and Sahin and Diwekar.[20]

The L-shaped BONUS algorithm is an integration of the traditional sampling-based L-shaped method and BONUS. The decomposition structure of the L-shaped algorithm is combined with the reweighting approach from BONUS to reduce the computations at the subproblem solution stage. The algorithm is explained below.

**2.4. Algorithm Structure.** The algorithm structure is shown schematically in Figure 5. The structure is based on the standard sampling-based L-shaped method with the incorporation of a reweighting scheme, which is part of the solution to the second-stage problem.[9]

The reweighting scheme, as mentioned previously, requires simulation results for the base case (uniform) distribution. For this purpose, during the first optimization iteration, the model is run for each sample to determine the output distribution of the model, which is called the base-case distribution. It is used to derive the feasibility and optimality cuts for the master problem and generate the upper bound on the objective function. However, during the second and subsequent iterations, the reweighting scheme, with Gaussian Kernel Density Estimation, is used to predict the probabilistic values (e.g., expectation) of the model output used to solve the second-stage dual problem. This procedure is continued until the termination criteria for the L-shaped method are met. The algorithm details can be found in the work by Shastri and Diwekar.[9]

The advantages of the L-shaped BONUS algorithm are as follows:

• The algorithm is computationally efficient, resulting in faster problem solutions. The effect is more pronounced for nonlinear and/or high dimensional models.

• The reweighting scheme does not assume linearity for uncertainty propagation. The ability of the reweighting scheme to estimate the probabilistic output of a nonlinear model reliably is a very important property. This property makes the L-shaped BONUS algorithm suitable to solve stochastic *nonlinear* programming problems.

• The algorithm is able to convert an SNLP problem to an SLP problem using reweighting to approximate nonlinear relationships.

• The algorithm can solve optimization problems using black-box simulation models. Off-line simulation results can be stored and used by the reweighting scheme to estimate the model results in the optimization procedure.

The computational properties of the algorithm are further enhanced by using the Hammersley Sequence Sampling technique to sample the uncertain parameters.[23,24] This sampling technique is shown to have superior $k$-dimensional uniformity properties in comparison to Monte Carlo (random) sampling and other stratified sampling techniques. Because the decomposition structure is based on the original L-shaped method, the requirement of problem convexity is maintained for the L-shaped BONUS algorithm.

The next section presents the Christina River watershed nutrient management problem, where pollutant trading has been proposed as a management alternative. To facilitate understanding of the problem, the basics of pollutant trading are initially reviewed, followed by the presentation of the watershed details. The analysis of the problem motivates the formulation of a nonlinear stochastic programming problem for optimizing trading decisions. The proposed L-shaped BONUS algorithm is then used to solve this problem in a computationally efficient manner. The results are used to compare the proposed algorithm with the standard L-shaped method.

## 3. Pollutant Trading: Christina River Watershed Case Study

**3.1. Basics of Pollutant Trading.** Environmental credit trading is an approach to environmental protection that uses market-based mechanisms to efficiently allocate emission or pollutant reductions among sources with different marginal control costs. The goal is to attain the same or better environmental performance with respect to pollution management at a lower overall cost. Pollutant trading adds flexibility and introduces new options to the policy makers and industries alike. After the early applications designed to provide greater flexibility for emission sources to meet air quality standards in a cost-effective manner,[11,25−28] trading principles have been sanctioned by USEPA for water pollution problems on a limited basis since the early 1980s. Trading is based on the fact that sources in a watershed can face very different costs to control the emission

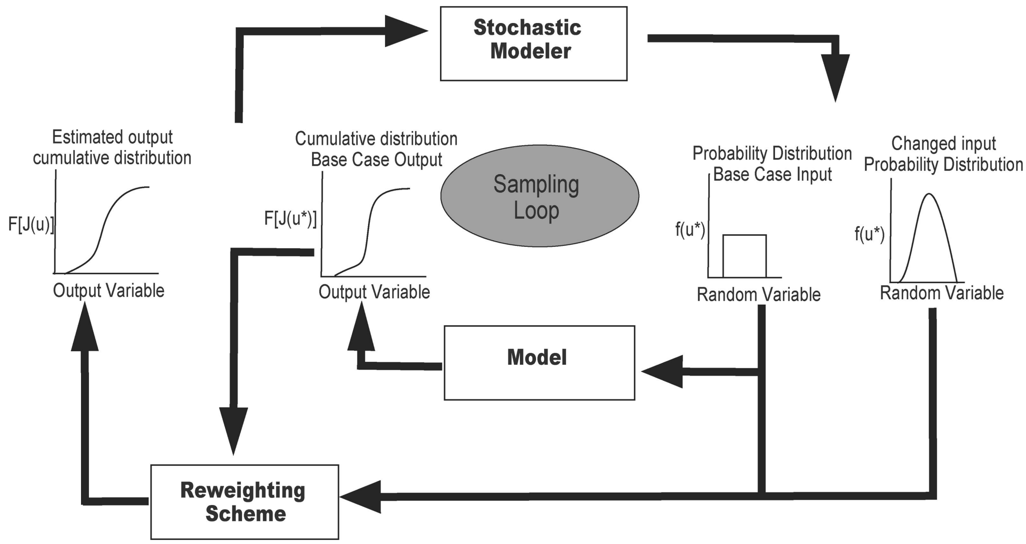


Figure 4. Reweighting approach in BONUS.

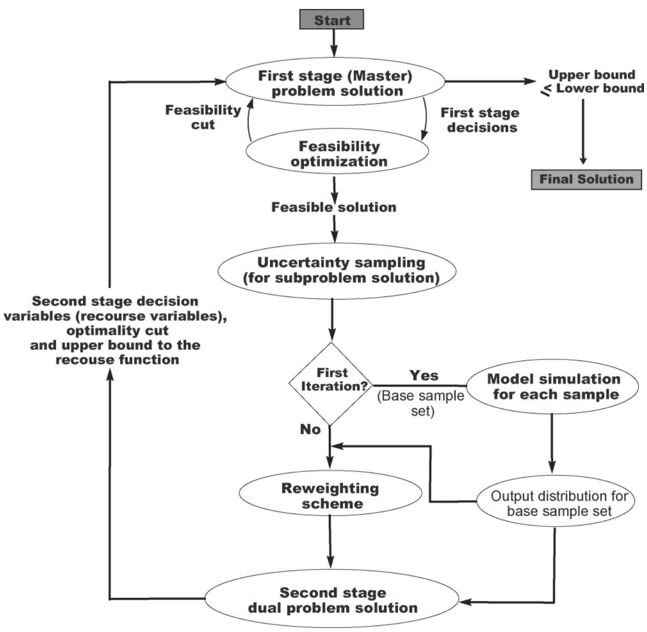


Figure 5. The L-shaped BONUS algorithm structure.



of the same pollutant. Trading programs allow facilities facing higher pollution control costs to meet their regulatory obligations by purchasing environmentally equivalent (or superior) pollution reductions from another source at a lower cost. Firms that have financial capabilities and infrastructure to perform pollutant reduction below the required limit get credits for it, which can be sold to another firm to gain monetary benefits.

Various aspects of watershed based trading are discussed extensively in USEPA technical reports from 1996[29] and 2003,[30] and only the highlights are presented here. The state or federal authority proposes a regulation such as the total maximum daily load (TMDL), which establishes the loading capacity of a defined watershed, identifies reductions or other remedial activities needed to achieve water quality standards, identifies sources, and recommends waste load allocation for various polluters. To comply with the regulation, a polluter may be required to reduce its discharge level. It has two options to accomplish this:

(1) The polluter can implement end-of-pipe treatment methods, which entail certain capital and operating costs, depending on the existing technology, the amount of waste being treated, and the level of reduction being achieved. These costs typically differ for different polluters.

(2) The polluter can trade a particular amount of pollutant to another source in the watershed that is able to reduce its discharge more than that specified by the regulation.

Various parameters that affect the economics of trading are trading ratio (how many units of pollutant reduction a source must purchase to receive credit for one unit of load reduction), transaction costs (expenses for trading participants that occur only as a result of trading), number of participants, availability of cost data, and uncertainties related to continued industry participation and data availability.

A polluter is mainly classified as either a point source or a nonpoint source. Point source (PS) is defined as those that have direct and measurable emissions (such as industries), while nonpoint sources (NPS) with diffused emissions that are difficult to measure (such as agricultural runoffs). Such varying pollutant sources result in different possible ways to practice pollutant trading.[29,31] Of these, trading between point and nonpoint sources is considered to have the greatest potential for water pollution control.[32] This is because nonpoint sources are the primary polluters, from a volumetric perspective, in most water bodies. Moreover, pollution abatement costs for the nonpoint sources (through best management practices (BMPs)) are quite often considerably lower than those for point sources. However, the nonpoint sources are associated with uncertainties that complicate the problem solution. First of all, contributions from nonpoint sources are not accurately measurable (at a reasonable cost), and because the contributions are diffused, the effect of the pollutant reduction strategies is also difficult to estimate. Furthermore, contributions from many of the nonpoint sources are dependent on essentially stochastic factors, such as rainfall and weather conditions.[29,32]

Thus, in the presence of multiple polluters (point sources as well as nonpoint sources), and uncertainties associated with the nonpoint sources, heuristics-based decision making can be suboptimal. A systematic framework, based on sound mathematical modeling concepts, can be an invaluable tool to the industries to analyze various options and optimize their decisions. The problem discussed in this work is a step in that direction. It proposes to use optimization theory as the decision making tool. The next section presents the Christina River watershed case study, followed by the formulation of the trading problem.

**3.2. Christina Watershed Nutrient Management.** The Lower Delaware River (LDR) Basin has been investigated in the past because of its problems with respect to point as well as nonpoint source pollution.[33] In the LDR, industrial discharges, urban runoff, and agriculture are the major causes of impairments, and in the state of Pennsylvania itself, over 156 segments of water bodies have been identified as being impaired. Sediments and nutrients are the major sources of concern in these segments.[33] Authorities have developed multiple TMDLs, targeting different pollutants and different geographical locations for the impaired LDR Basin. A review of those TMDLs can be found in Scatena.[33]

The Christina watershed is an important watershed in LDR. The watershed drains three states and provides up to 100 million gallons of public drinking water per day.[34] The Christina River, Brandywine Creek, Red Clay Creek, and White Clay Creek are the major waterways within the basin. However, various segments of the basin have been declared as being impaired. Thirty nine segments of the basin have been declared as being impaired because of low levels of dissolved oxygen (DO), and nutrient additions from various point and nonpoint sources are considered to be the major cause. The important sources of pollutants and water quality degradation within the basin include industrial and municipal point sources, agriculture, superfund sites, and hydromodifications.[35] Authorities have proposed two different TMDLs for the watershed. The low-flow TMDL focuses on the impact of nitrogen and phosphorus additions from the point source permit holders,[35] whereas the high-flow TMDL accounts for the nonpoint source additions of bacteria and sediments.[36] This work considers the low-flow TMDL targeted to achieve acceptable DO levels through PS load allocations for total phosphorus, total nitrogen, ammonia nitrogen, and carbonaceous biochemical oxygen demand (CBOD). Trading has been proposed as being a viable option to achieve the reduction goals.

Although trading between various PS is the simplest trading mechanism, opportunities in the watershed are limited because of similar treatment costs throughout the watershed. However, there are significant opportunities for trading between point and nonpoint sources.[33] Nonpoint sources of pollution mainly include various agricultural runoffs, which cause nutrient addition to the watershed. Therefore, converting existing agricultural land to forest or establishing BMPs on the cultivated land is a possible option.[33] Here, a particular land will be allocated to a particular PS through a trading mechanism and the PS will be responsible for the management of the NPS to offset nutrient discharges from the PS facility. This is the basic trading mechanism that has been analyzed in this work.

The basics of watershed based pollutant trading and Christina watershed nutrient management problem presented in the preceding sections form the basis of the optimization trading problem formulation explained in the next section.

**3.3. Trading Problem Formulation.** The literature on modeling of point/nonpoint water pollutant trading is diverse, with the focus varying from regulations to economics.[37−39] The trading model used in this work is based on the models proposed in Malik et al.[37] and Zhang and Wang.[40] Initially, a general problem applicable to any watershed is formulated, which is then applied to the Christina watershed case study. The presence of uncertainty associated with the nonpoint sources necessitates the formulation of a stochastic programming problem. The solution of this stochastic programming problem is achieved using the proposed L-shaped BONUS algorithm.

The problem considers trading between a set of point sources (PS) and one nonpoint source (NPS), representing a farm. All these sources discharge the pollutants into a common body of water, such as a lake. Regulations have been placed on the discharge of a set of chemicals, specifying the maximum amount that is allowed to be discharged per day into the body of water. Currently, the NPS are not regulated, because it is not possible to measure the emissions from these sources accurately. For simplicity, this model does not consider regulations on NPS emission. The development of TMDL results in specific load allocations that are used as the basis of trading between the PS and the farm (NPS), as explained previously. Note that the reduction techniques for the farm are dependent nonlinearly on the type and quantity of chemical being treated.

There are three sources of uncertainty in this setup. As mentioned previously, the NPS have uncertain emission quantities and uncertain reduction efficiencies for a particular technology. These two factors combine to give variability in the actual reduction achieved by BMP for a particular chemical. Although PS generally have measurable discharge quality and quantity, these can additionally be associated with some uncertainty. An example of this is a publicly owned water treatment plant (POWT). A POWT is a state- or municipality-owned wastewater treatment facility that is designed to treat a variety of pollutants, such as sewage waste, water runoffs, and others. Although POWT is a PS in terms of the output concentration of the chemicals, the total amount of waste being discharged is subject to variability. This is because a POWT often treats wastes from many disparate sources, some of which are stochastic in nature. As a result, the amount of input and, consequently, the output varies within certain limits. This constitutes the third uncertain parameter in the problem.

Let $i = 1,..., P$ represent the set of PS, and $j = 1,..., M$ represent the chemicals that are regulated. For the PS, the current pollutant discharge levels are known, along with the discharge reduction (treatment) cost for all the chemicals. The model parameters associated with the PS include the following: $D(i)$, which is the total volumetric discharge from point source $i$ (expressed as $[L^3]/[s]$); $e_{p0}(i,j)$, which represents the pretreatment discharge quantity of chemical $j$ from point source $i$ (expressed as $[M]/[L^3]$); and $c_p(i,j)$, which represents the cost for the point source discharge reduction of chemical $j$ by point source $i$ (expressed as [$]/[M]). [Here, the terms in brackets represent the dimensions of various quantities: [M] = mass, [L] = length, [s] = time, and [$] = cost (in dollars).]

For the NPS, it is considered that a fixed amount of land is available that can be divided among all PS to implement treatment technologies (BMP). Similar to the PS, current discharge quantities, discharge reduction costs, and abatement efficiencies are known for the NPS. The model parameters associated with the nonpoint source include the following: $L_{max}$, which is the maximum amount of NPS land available for trading (expressed as $[L^2]$); $e_{n0}(j)$, which represents the pretreatment discharge quantity of chemical $j$ from the NPS (expressed as $[M][L^2][s]^{-1}$); $c_n(j)$, which is the cost for the NPS discharge reduction of chemical $j$ (expressed as $[\$][L^2]^{-1}$); $b_{NPS}(j)$, which represents the NPS abatement efficiency of chemical $j$; and $q_n(j)$, which is the abatement in NPS discharge of chemical $j$ (expressed as $[M][L^2][s]^{-1}$). [Here, $q_n(j) = e_{n0}(j)b_{NPS}(j)$.]

From the regulatory perspective, in addition to the waste load allocations for different PS, there are restrictions on the maximum amount of any chemical that can be discharged into

**Table 1. PS Details for Christina River Basin**

| | | Current Discharge (kg/day) | | Targeted Reduction (%) | | Treatment Cost ($/kg) | |
|---|---|---|---|---|---|---|---|
| point source | total discharge (MGD[a]) | nitrogen | phosphorus | nitrogen | phosphorus | nitrogen | phosphorus |
| 1 | 0.4 | 30.30 | 30.30 | 0 | 13 | 15.6 | 5.2 |
| 2 | 1.028 | 233.63 | 38.94 | 26 | 26 | 14 | 4.9 |
| 3 | 7.5 | 568.18 | 568.18 | 25 | 0 | 10.9 | 3.8 |
| 4 | 3.85 | 291.66 | 299.76 | 0 | 28 | 12.7 | 4.2 |
| 5 | 0.6 | 68.18 | 45.45 | 10 | 10 | 15.4 | 5.1 |
| 6 | 1.1 | 125.0 | 313.72 | 34 | 83 | 14.4 | 5 |
| 7 | 0.72 | 5.45 | 5.45 | 5 | 5 | 18.3 | 5.4 |
| 8 | 0.7 | 171.06 | 26.51 | 69 | 0 | 15.4 | 5.12 |

[a] MGD = millions of gallons per day.

the water body at a particular location. Enforcing this limit ensures that the implementation of pollutant trading does not result in the creation of "hot spots", which are defined as localized points with high pollutant concentration. Accordingly, the regulatory parameters of the model are $z_{\text{red}}(i, j)$, which represents the targeted reduction in discharge of chemical $j$ by point source $i$ (expressed as $[\text{M}][\text{s}]^{-1}$), and $z_{\text{allowed}}(j)$, which is the maximum permitted discharge of chemical $j$ at any location (also expressed as $[\text{M}][\text{s}]^{-1}$).

In the context of sources of uncertainty previously described, parameters $e_{p_0}(i,j)$, $b_{\text{NPS}}(j)$, and $D(i)$ are uncertain. The decisions to make are as follows:

• Should pollutant quantity be traded with the land (nonpoint source (NPS)), and, if so, how much?

• How much reduction should be achieved by the end-of-pipe treatment, with the objective of achieving the reduction targets at the lowest *overall* cost?

Accordingly, the decision variables in the model are $L(i,j)$, which represents the land allocated for trading by point source $i$ to treat chemical $j$ (expressed as $[\text{L}^2]$), and $q_p(i,j)$, which represents the discharge abatement of chemical $j$ by point source $i$ using the end-of-pipe treatment (expressed as $[\text{M}][\text{L}^3]^{-1}$).

The uncertainties associated with the problem necessitate the formulation of a stochastic programming problem, which is given as follows:

$$\text{Min}\, f_1(c_n, L) + E[f_2(D, c_p, q_p)] \tag{6}$$

where $E$ is the expectation operator over the uncertain parameters and $f_1$ and $f_2$ are linear/nonlinear functions of the respective variables. The first term in the objective represents the cost incurred due to trading through the allocation of land for each PS from the NPS. The second term represents the expected value of the total treatment cost incurred by the PS to satisfy the regulations in the presence of uncertainty. This objective is subjected to the following constraints:

$$\sum_{i,j} L(i, j) \le L_{\max} \tag{7}$$

$$E[D(i,j)q_p(i,j) + L(i,j)q_n(j)] \ge z_{\text{red}}(i,j) \qquad \forall\,(i,j) \tag{8}$$

$$E[D(i,j)(e_{p_0}(i,j) - q_p(i,j))] \le z_{\text{allowed}}(j) \qquad \forall\,(i,j) \tag{9}$$

$$0 \le q_p(i,j) \le e_{p_0}(i,j) \qquad \forall\,(i,j) \tag{10}$$

$$q_n(j) = e_{n_0}(j) b_{\text{NPS}}(j) \qquad \forall\,(j) \tag{11}$$

The first constraint ensures that the total land allocation does not exceed the amount of land available with the NPS. The second set of constraints ensures that each industry achieves the individual reduction target of each chemical, with or without trading. The third set ensures that the emission of a pollutant $j$ at any location does not exceed the permitted value. Constraint 10 bounds the PS reduction. The last constraint models the effect of uncertainty on the problem. The terms $e_{n_0}(j)$ and $b_{\text{NPS}}(j)$ are uncertain parameters that affect pollutant reduction by the NPS ($q_n(j)$).

The problem can be converted to a two-stage stochastic programming problem with recourse, where the first-stage decisions are the land allocations between various PS and the NPS $L(i, j)$, and the second-stage decision variables are the PS abatement $q_p(i,j)$ to be achieved by the end-of-pipe treatment, to take care of the uncertainties. The two-stage formulation, where specific definitions of functions $f_1$ and $f_2$ are also included, is given below:

*First-stage problem:*

$$\text{Min} \sum_{i=1}^{P} \sum_{j=1}^{M} c_n(i,j) L(i,j)^{\alpha_j} + E[R(L, q_p, q_n, D)] \tag{12}$$

$$\sum_{i=1}^{P} \sum_{j=1}^{M} L(i, j) \le L_{\max} \tag{13}$$

where, $R$ is the recourse function. The term $\alpha_j$ is a constant for chemical $j$, that represents the nonlinear relationship between land allocation and pollutant reduction.

*Second-stage problem:*

$$\text{Min}\, E[R(L, q_p, q_n, D)] = \sum_{n=1}^{N} \sum_{i=1}^{P} \sum_{j=1}^{M} D(i,j,n) c_p(i,j) q_p(i,j,n) \tag{14}$$

$$D(i,j,n)q_p(i,j) + L(i,j)q_n(j,n) \ge z_{\text{red}}(i,j,n) \qquad \forall\,(i,j,n) \tag{15}$$

$$D(i,j,n)[e_{p_0}(i,j) - q_p(i,j,n)] \le z_{\text{allowed}}(j) \qquad \forall\,(i,j,n) \tag{16}$$

$$0 \le q_p(i,j) \le e_{p_0}(i,j) \qquad \forall\,(i,j) \tag{17}$$

$$q_n(j,n) = e_{n_0}(j) b_{\text{NPS}}(j,n) \qquad \forall\,(j,n) \tag{18}$$

where $N$ is the sample size used to represent the uncertain space in the optimization algorithm, and $n$ is a particular sample from the uncertain space. Equations 12−18 represent the general two-stage stochastic programming problem with recourse.

For the Christina watershed, the authorities have recommended 8 PS for trading, out of a total of 104 PS. Two PS of the selected eight are private industries, whereas the remainder are municipal polluters (such as POWT). This work includes these eight PS in the trading problem. Two nutrients (nitrogen and phosphorus) are considered as the tradable commodities. TMDL-generated reduction targets for each PS are known for both nutrients. The total volumetric discharge, as well as the current discharge levels and reduction targets for both pollutants, are taken from the USEPA[41] and are given in Table 1. (Note that the values of current discharge are derived from the percentage reduction targets and waste load allocations.) The cost of nutrient reduction through the installation of the end-

**Table 2. Details of Non-Point-Source Emission and Treatment**

| | nitrogen | phosphorus |
|---|---|---|
| mean value of emission quantity (kg per unit area per day) | 20.2 | 30.5 |
| standard deviation in emission quantity | 2.0 | 2.0 |
| BMP cost ($ per unit area) | 17.18 | 17.18 |
| BMP nutrient reduction efficiency | 0.50 | 0.39 |
| standard deviation in reduction efficiency | 0.02 | 0.02 |

of-pipe treatment has been reported for Chesapeake Bay (http://www.chesapeakebay.net). The average cost of reduction for nitrogen and phosphorus is $15.62/kg and $4.46/kg, respectively. The actual costs for each PS have been assumed around the basic values and reported in Table 1. The second point source is considered to have uncertain volumetric discharge ($D(i)$). It is assumed to be normally distributed with a standard deviation of 0.025 (in MGD). Various BMPs for the NPS, along with the reduction efficiency and costs for nitrogen and phosphorus removal, are given in Scatena.[33] Because no particular BMP was known to be better-suited for the Christina Basin, this work uses the average values; these values are reported in Table 2. Also reported in Table 2 are the average discharge of both nutrients from the NPS prior to trading or BMP installation. The maximum allowed concentration of both nutrients at a particular discharge point in the watershed ($z_{\text{allowed}}$) is 450 and 570 kg/day for nitrogen and phosphorus, respectively. The total quantity of land available for trading ($L_{\max}$) is 500 units. Although some data for the problem is based on assumption, it has been selected to depict a typical tradeoff that is often observed in reality. The next section presents the results for the Christina watershed nutrient trading.



## 4. Results and Discussion

The objective of this work is to solve the trading problem and perform a comparative study of the L-shaped BONUS algorithm with the standard L-shaped method. Because the sampling technique has an important role in the sampling-based algorithms, a comparative analysis between the Hammersley Sequence Sampling technique (HSS) and the Monte Carlo sampling technique (MCS) is also performed. Accordingly, the problem is solved using four different methodologies:

- Standard L-shaped method with HSS
- Standard L-shaped method with MCS
- L-shaped BONUS method with HSS
- L-shaped BONUS method with MCS

The four methodologies are compared by studying the problem solution as a function of sample size, and the sample size is varied from 25 to 300. The variation of the objective function for the four methods is shown in Figure 6, while the typical variation of the decision variables is shown in Figure 7, which represents the land allocation decision by PS 8 toward nitrogen pollution trading.

Figure 6 indicates that the difference in the results for the two methods is within reasonable limits. The average difference between the objective function values for the two methods is 1.05% and 1.19% for HSS and MCS, respectively. This indicates that the reweighting approximation does not sacrifice accuracy. Also evident from the plots is the fact that the two solutions approach a steady-state value as the sample size is increased. The plot for the decision variable shows a similar qualitative behavior. The average difference between the two methods is even less for the decision variable plotted in Figure 7 (0.05% for HSS and 0.26% for MCS). A comparison of the two

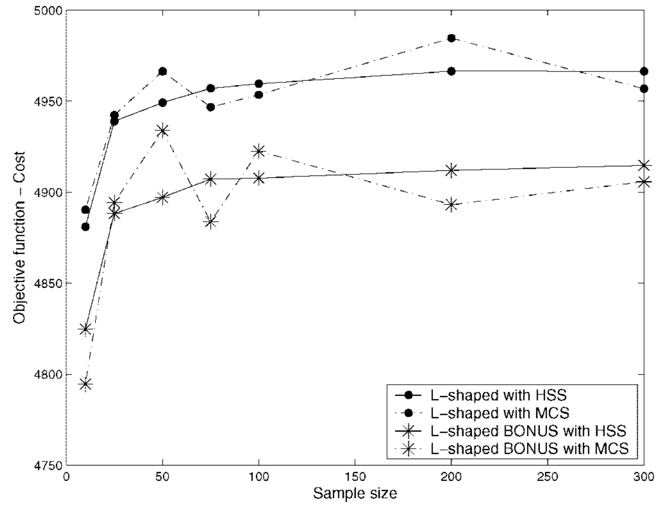


**Figure 6.** Variation of the objective function result with sample size.

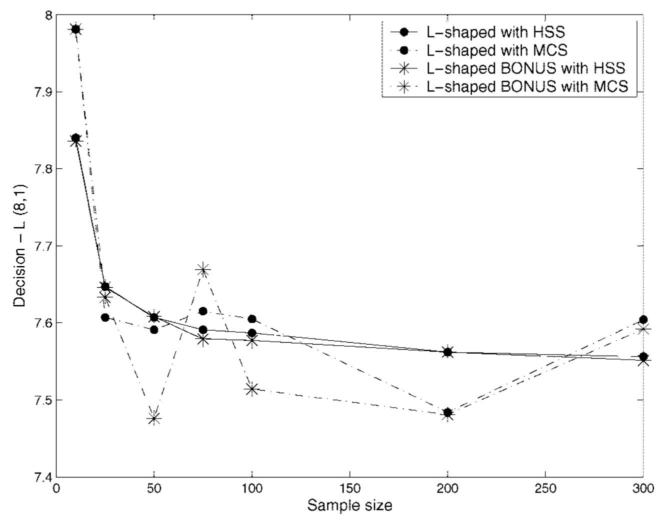


**Figure 7.** Variation of the decision variable 3 result with sample size.

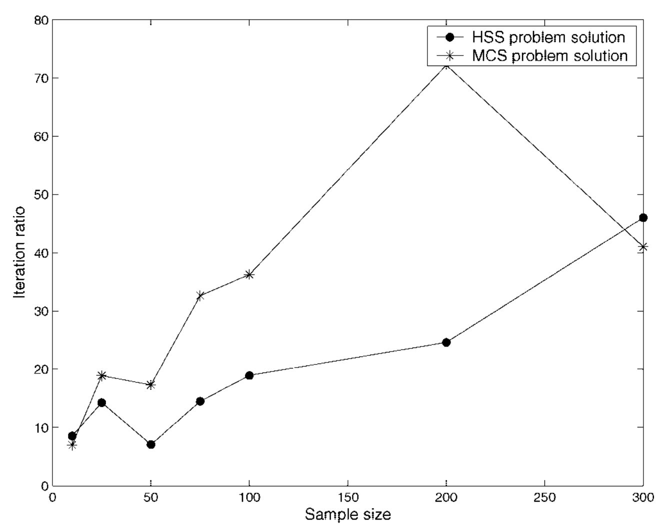


**Figure 8.** Variation of the computational time with sample size.

sampling techniques indicates that the results with the HSS technique reach the steady-state value faster as the sample size is increased than for the MCS technique. Also the error between the results for the two methods is smaller for the HSS technique, particularly at smaller sampling sizes.

**Table 3. Problems Solved Using L-Shaped BONUS Algorithm**

| | farmer's problem | chemical blending problem | sensor placement problem |
|---|---|---|---|
| aim | maximize profit | minimize blending cost | minimize risk due to contamination attack |
| decisions | planting strategy for the crops | blending strategy of the basic components | sensor locations in the network |
| nonlinearity | relationship between atmospheric parameters and seasonal yield | relationship between fraction of impurity and total impurity parameter | relationship between nodal demands and network flow patterns |
| uncertainty | atmospheric parameters | individual impurity fraction | nodal demands in the water network |

**Table 4. Comparison of the Results of Different Problems Solved Using the L-Shaped Method and the L-Shaped BONUS Algorithm**

| | Results | | | |
|---|---|---|---|---|
| | Number of Iterations/CPU Time (s) | | Objective Function Value | |
| sample size | L-shaped | L-shaped BONUS | L-shaped | L-shaped BONUS |
| | Farmer's Problem | | | |
| 100 | 26/NA | 7/NA | 122804 | −123513 |
| 200 | 38/NA | 7/NA | −122997 | −125840 |
| 300 | 45/NA | 7/NA | −123012 | −125872 |
| 400 | 25/NA | 7/NA | −123077 | −125356 |
| 500 | 54/NA | 7/NA | −123109 | −125224 |
| Other advantages: Converts a stochastic nonlinear programming (SNLP) problem into a stochastic linear programming (SLP) problem | | | | |
| | Chemical Blending Problem | | | |
| 100 | 11/16.32 | 2/1.98 | 64980 | 66054 |
| 200 | 9/25.84 | 2/4.54 | 64979 | 66027 |
| 300 | 6/26.59 | 2/7.12 | 64977 | 66010 |
| 400 | 5/29.64 | 2/10.03 | 64977 | 66006 |
| 500 | 6/43.71 | 2/13.28 | 64976 | 66003 |
| Other advantages: Converts a stochastic nonlinear programming (SNLP) problem into a stochastic linear programming (SLP) problem | | | | |
| | Sensor Placement Problem | | | |
| 100 | NA[a] | 11 | NA[a] | $1.145 \times 10^7$ |
| Other advantages: Allows the use of black-box simulation models in optimization algorithm | | | | |

[a] Not solved using the L-shaped method: black-box EPANET model simulation is needed for the subproblem solution for each sample.

An important advantage of the L-shaped BONUS algorithm is its computational efficiency due to the reweighting scheme. The problem solutions indicate that there is a significant difference between the solution times for the two methods, using both sampling techniques. Figure 8 plots the ratio of the computational time for the standard L-shaped method and the L-shaped BONUS algorithm. It can be seen that the value of the ratio increases as the sample size increases. Thus, the advantage becomes more obvious at larger sample sizes. Also observed is the fact that the ratio for MCS is higher than that for HSS. This means that the use of HSS leads to better computational properties when used with the proposed L-shaped BONUS algorithm. In the next section, a summary of results for the other problems solved by the L-shaped BONUS algorithm is given. These results, along with those for the presented trading problem, are used to draw conclusions in section 5.

With regard to the trading problem, the solution indicates that all PS need to achieve part of the required reductions through trading with the NPS to minimize the overall cost. Such a decision will be difficult to make if the industries make decisions on their own, without the consideration of the overall cost. Therefore, the results strongly support the use of a rigorous and systematic mathematical analysis to perform decision making in trading because the decisions based on heuristics are likely to be suboptimal.

**4.1. Summary of Algorithm Applications.** The previous section presented the pollutant trading problem and discussed the performance of the L-shaped BONUS algorithm to solve that problem. The algorithm has also been used to solve other problems of varying nature and dimension. These problems include an illustrative farmer's problem, a process-systems-engineering-relevant chemical blending problem,[9] and a large-scale problem of sensor placement in water distribution networks.[10] The sensor placement problem also highlights the ability of the algorithm to use black-box simulation models in thr optimization procedure. The objective is to investigate the performance of the algorithm in solving examples of differing nature. Table 3 gives the important information about these problems. The detailed problem description, found in Shastri and Diwekar[9] and Shastri and Diwekar,[10] has been omitted here for the sake of brevity. A summary of the results for these problems is reported in Table 4. The table illustrates that these results are qualitatively similar to those obtained for the trading problem presented in this paper. The next section uses these observations to draw conclusions.

## 5. Conclusion

This paper has discussed the application of a recently proposed L-shaped BONUS algorithm to solve stochastic nonlinear programming (SNLP) problems on an environmental trading problem of nutrient management in the Christina River Basin of the Lower Delaware River. The environmental trading problem is formulated as a two-stage stochastic programming problem, making it amenable to specialized stochastic programming solution methods such as the L-shaped method. The new algorithm, which is an integration of the BONUS algorithm and the traditional L-shaped method, is stated to provide computational benefits for solution of large-scale nonlinear stochastic problems. The properties of the environmental trading problem solution lend support to this argument by showing that the L-shaped BONUS algorithm is computationally much more efficient, compared to the sampling-based L-shaped method. At the same time, the L-shaped BONUS algorithm does not compromise result accuracy, as indicated by a <2% difference in the final result in most cases. Furthermore, based on the summary of results presented in Table 4, the following general conclusions about the algorithm can be drawn:

The L-shaped BONUS algorithm:

• Solves SNLP problems

• Exhibits computational efficiency, because of (i) the decomposition structure from the L-shaped method, (ii) the reweighting scheme from the BONUS algorithm in the stochastic modeler, (iii) efficient sampling from HSS, and (iv) conversion to linear problems

• Converts SNLP problems to stochastic linear programming (SLP) problems

• Can use off-line simulations for the (nonlinear) models (black-box simulators)

From a trading perspective, the potential of water pollutant trading between point sources (PS) and nonpoint sources (NPS) is well-known. However, as the problem formulation and the results suggest, decision making in point/nonpoint trading is complex and requires a systematic analysis. The existence of various tradeoffs and restrictions make it an ideal problem for the optimization theory. The presented work is the first instance of the formulation of a point/nonpoint trading problem using stochastic programming ideas. Advances in the field of stochastic programming offer an exciting avenue to make better decisions in the goal of environment preservation. It is expected that efficient decision making in such matters will be important for the sustainability of chemical process industries in future. In this regard, further investigations into a more-detailed analysis of stochastic programming applications in environmental trading problems offers considerable prospects.

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