WATERSHED MANAGEMENT AND WATER QUALITY TRADING:

A SYSTEMATIC FRAMEWORK FOR ASSESSING UNCERTAINTY

by

FENG SHI

(Under the direction of M. Bruce Beck)

ABSTRACT

Uncertainty in our knowledge of the behavior of environmental systems should be fully addressed and properly accounted for, if we are to have effective and reliable environmental policies. To that end, a systematic framework for watershed modeling and the analysis of uncertainty is proposed and presented in this dissertation. The framework houses several major components: a watershed simulation tool, itself composed of several parts; algorithms for the analysis of uncertainty and sensitivity; and assessment of the economics of water quality trading. Central to the analysis of uncertainty is a sampling-based approach based on what is familiarly known as a Regionalized Sensitivity Analysis. A case study is employed to illustrate the capabilities of the proposed framework. First, the problem of model identification from field data – under uncertainty – is discussed. Second, a more comprehensive watershed model is assembled in order to study two important aspects of water quality management in a significant portion of the Chattahoochee watershed, including the Metropolitan Atlanta area, again focusing on the nutrient phosphorus. Significantly, the watershed model treats the dynamic behavior of both nonpoint- and point-source discharges of phosphorus on a compatible basis. In the first part of this case study, suitable regulatory standards for water quality are used to develop a TMDL for phosphorus, which is allocated amongst the nonpoint and point sources in the watershed. The Chattahoochee case study is then completed with a more advanced analysis of nutrient trading, between point- and nonpoint-source dischargers. Feasibility and desirability of any such trading scheme are assessed according to the dual measures of economic surplus in the potential trading market and improvement in water quality. All the uncertainties involved, both scientific and economic, are evaluated by means of the sampling-based RSA algorithm. Since uncertainty is conventionally handled through a rather crude choice of a Margin of Safety in setting TMDL policies, and through the so-called "trading ratio" crucially for the design of effective water quality trading policies, the Chattahoochee case study realistically address two important contemporary problems. The dissertation argues that its proposed approach to the analysis of uncertainty in such matters is an important contribution to the design of reliable environment policies in the future.

INDEX WORDS: Watershed Modeling, Uncertainty Analysis, Water Quality Trading, TMDL, RSA, Chattahoochee River

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With love and devotion to Jessica, Selina and Great Zuguo, who make all these efforts meaningful.

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INTRODUCTION

1.1 Background

1.1.1 Science and environmental management

Environmental management is the management of human interaction with, and impact upon, the environment, for better utilizing and conserving natural resources and the environment and realizing sustainability. For the past several decades, we have witnessed in the field of environmental research that scientific studies are extensively conducted for the purpose of underpinning practical environmental management. In order to ensure that environmental policies are developed and applied in a valid and effective way, sufficient scientific explorations are required as a basis for decision-making. Currently the trend towards greater interaction between environmental science and management is becoming increasingly significant (King and Corwin 1999). On the one side, we see that the task of policy development provides great incentives for the relevant scientific research; on the other, the unprecedented advancement of science and technology are making greater contributions in many aspects of environmental management, as well as stimulating new public policy debates. Consequently, a concept of scientific environmental management is introduced here. By "scientific environmental management" we mean that environmental management strategies are developed and evaluated based on adequate and appropriate scientific studies, which include, yet are not limited to, comprehensive investigation of the given environmental system; application of quantitative and scientific approaches for accurate system analysis, assessment and forecasting, and an appropriate evaluation of the associated uncertainties or risks. All of these efforts are aimed at enabling environmental management to be effective, efficient and reliable.

With respect to water resources and water quality management at the watershed scale, we see the paradigm of closer policy-science relations as well. For example, the nation-wide promotion of pollution control programs such as TMDL (Total Maximum Daily Load) has significantly stimulated the application of watershed models to estimate the pollution yield and to simulate the fate of these pollutants in the receiving waterbody. At the same time, advanced techniques such as automated sampling and monitoring, quantitative analysis approaches (including modeling and statistical analysis), information and computer techniques, are all substantially contributing to the processes of policy development.

In particular, as the most important tool to support environmental management, mathematical models are playing an indispensable role in providing quantitative information to devise alternative pollution control strategies. In recent watershed studies, for better exploring and understanding the behavior of the complex watershed system, so-called "mechanistic" models are being used with increasing frequency to simulate the hydrologic and pollutant transport processes. Specifically, in order to support watershed environmental management, we need to make accurate assessment and prediction of the pollutant yield and resultant instream water quality. With the assistance of models, we are able to achieve a quantitative understanding and description of the behavior of the watershed system and thus place our decisions on a more scientific substrate. In addition, watershed models are also used to forecast the water quality response to external factors, including natural variations in the system, development scenarios, and policy implementation, for providing scientific support for associated watershed planning and management issues.

Furthermore, due to the high complexity of an environmental system, the inherent uncertainty needs to be sufficiently accounted for, to assure the reliability of environmental studies and practical management programs. We have noticed that the issue of uncertainty has important policy, regulatory, and management implications, especially when models are employed. Uncertainty analysis (UA) is an indispensible scientific tool to ensure the quality of environmental modeling or assessment, and consequent environmental management. In fact, our understanding of the environmental system, such as a watershed, is often expressed by means of the combination of dynamic simulation and uncertainty analysis, where the model describes the internal process mechanism, in the relationships between variables, whose trustworthiness is evaluated by UA. Accordingly, in order to achieve the so-called scientific management of the environment, decisions must be made on the basis of sufficient and proper understanding of the given environmental system, and for this purpose, with the support of a mathematical simulation model and involvement of scientific assessments of the uncertainties (Reckhow 1994). Additionally, environmental or ecological risk assessment is a typical way of indicating how scientific thinking can improve the effectiveness of decisions (NRC 1999). Since we have also noticed that systematic uncertainty assessments are rarely conducted, especially for decision-oriented modeling studies, this remains a big challenge in the field of environmental study (Beven 2008; Pappenberger and Beven 2006; Zheng and Keller 2007).

Therefore, in this dissertation we will mainly focus on two main topics, modeling and uncertainty analysis, and explore their roles, interactions, and joint contributions in watershed and water quality studies, whilst yet being highly attuned to the political context of watershed management.

1.1.2 Toward an interdisciplinary research

Our object of study is a complex natural-social-economic system that contains multiple components, such as natural hydrological processes, human activities, and management issues. Accordingly, techniques from different disciplines are required to be synthesized for achieving the holistic study of an environmental systems analysis. This must combine and communicate knowledge from the natural and social sciences, with that of technology. Being interdisciplinary is one of the inherent features of environmental studies, especially for those that are management-oriented, because no matter how promising an innovative management tool is for benefiting the environment, its adoption is highly unlikely to occur without social legitimacy and economic feasibility being accorded to it (Rhoten and Parker 2004). A multidisciplinary approach, combining both environmental and economic analyses, is a good direction for improving environmental decision-making at the watershed level. It is also considered as a tendency of modern science advancement, notwithstanding many practical and philosophical obstacles, which exist and constrain such interdisciplinary environmental research (Campbell 2005; DeBarry 2004).

Moreover, we believe that the ultimate aim of environmental management is to achieve the sustainability, for not only the natural system, but also society and the economy. With respect to the topic of sustainability, beyond the original definition by Brundtland, “meeting the needs of the present without compromising the ability of future generations to meet their own needs", the framework of the triple bottom line, i.e. "being environmentally benign, economically feasible, and social legitimate", brings a more specific perspective to gauging sustainability in the water sector (Beck 2008; Elkington 1998). If the triple bottom line is to be employed, adopting a multi-disciplinary perspective herein becomes even more necessary and appropriate. Facing the interdisciplinary problem of watershed research, we are inevitably required to synthesize the methodology from environmental science, engineering, economics and sociology, although the sophisticated political issues will not be a focus in this dissertation.

1.2 Objectives and main content

The overall goal of this research is to develop a computational framework for quantitatively characterizing a watershed system, and providing substantial support for the decision-making process in environmental management. Modeling and uncertainty analysis are the two key components in this framework. Herein we will discuss two typical management tools, the TMDL and water quality trading. Our purpose is to illustrate how decision making in watershed management can substantially benefit from a computational framework. Once constructed, this framework is applied to a significant portion of the Chattahoochee watershed around the metropolitan Atlanta area, in Georgia, the United States. Phosphorus, as the growth-limiting nutrient for eutrophication in lakes and reservoirs in the South Eastern U.S., and many places throughout the world, is chosen as the pollutant of concern.

Integration in this framework is demonstrated by the combination of the dynamic watershed model, an economic assessment component, and the uncertainty processing platform, named as the

Integrated Modeling under Uncertainty for Supporting Environmental Management (IMUSEM) framework. These three principal components are mirrored in the main content of this dissertation.

With respect to the modeling component, this body of work includes model construction, calibration, and evaluation, to illustrate how watershed models are applied to describe the complex environmental system quantitatively. With respect to the uncertainty component, this is present and prominent in each of the phases of modeling. The analysis of uncertainty herein is directed at developing a framework for comprehensively characterizing all the important sources of uncertainty and their interactions in management-oriented watershed modeling. A sampling-based approach is applied for quantifying the resultant uncertainty for complex watershed models, and subsequent watershed management strategies. More specifically, after a systematic investigation of the uncertainty in the process of management-oriented watershed modeling, the dissertation responds to the questions of how the uncertainty in the environmental system should be identified, and quantitatively assessed, to reveal its influence on modeling outcomes, as well as how it can be appropriately processed to restrain impairment of the reliability of watershed management practices. In the third component of our overall economic assessment, i.e., economic assessment, we will estimate the cost of pollution control practices, insert them into the framework for achieving a multidisciplinary environmental-economic study, identify and analyze the involved uncertainty, while estimating the financial benefit generated by the mechanism of a potential trading market. With this entire framework, a cradle-to-grave analysis of uncertainty, covering the monitoring data, environmental modeling, economic analysis, and management concerns, is achieved and illustrated.

To summarize, the dissertation explores how watershed models can be employed as a basis for watershed study, how (and how much) uncertainty will be involved in the development and application of watershed management policies, and how we can evaluate them to avoid, or lower, the risk of policy ineffectiveness. The essential thrust is towards constructing a solid base for supporting the decision-making process and achieving scientific watershed management.

Other facets of the multi-disciplinary composition of this dissertation include the following: the development of a mechanistic watershed model, drawing upon representations of the underlying hydraulic, chemical, and biological processes; during the uncertainty processing procedure, statistical approaches are called into play; and, finally, for the policy-supporting task, economic analysis is employed to assess the financial feasibility of environmental management practice. We believe that this research framework is particularly compatible with the rising focus on integrated water resources management, which incorporates quantitative evaluation and aims at protecting and improving water resources while considering economic and social concerns of the community.

1.3 Thesis structure

This dissertation comprises eight chapters. This first chapter is a brief introduction to the background and overall goals of the research and principle contributions of this dissertation.

Chapter 2 discusses the topic of watershed management, whose technical support requirements are the motivation for this research. An extensive review of two water quality management tools, the TMDL and water quality trading, concludes that uncertainty is significantly involved and needs to be properly addressed and accounted for, if we are to assure the effectiveness and reliability of environmental policies.

Given these issues of Chapter 2, Chapter 3 reviews the literature on the two scientific tools to be intensively employed in this thesis: watershed modeling and uncertainty analysis. The chapter concludes that a standard and systematic framework of modeling under uncertainty is urgently required.

Chapter 4 is an in-depth study of some technical matters underpinning the methodology of uncertainty and sensitivity analysis. The concept of regionalized sensitivity and a method for analyzing it are elaborated. Then focusing on the problem of numerical instability demonstrated by earlier research, the statistical attributes of the K-S (Kolmogorov-Smirnov) statistical index are explored and suggestions made for standardizing and generalizing application of this method as a universal approach. The Regionalized Sensitivity Analysis (RSA) approach is applied throughout this dissertation as a major tool of systems analysis.

In Chapter 5, a comprehensive watershed simulation system is assembled from a set of component models and applied to the large watershed of the Chattahoochee, so that the dynamic behavior of both point- and nonpoint-discharges of pollutants into the river system, as well as the in-stream routing processes, can all be simulated in a compatible manner. The stream component is calibrated against sparse monitoring data obtained from the Chattahoochee river, with an algorithm derived from RSA. This modeling study helps us to improve our understanding of the hydraulic and nutrient behavior of such a large watershed.

Chapter 6 introduces the modeling-under-uncertainty framework and its application to the case study of the Chattahoochee watershed. After evaluation of the major sources of uncertainty arising from natural factors, the simulation system is embedded in the sampling-based Monte Carlo framework in order to examine the impacts of these uncertainties on simulation results: the distributions of instream water quality and nutrient loads. Based on the computational work, the TMDL for this watershed is evaluated in a scientific and reliable manner.

In Chapter 7 we propose and undertake a wider integrated analysis associated with exploring the other more complicated watershed management policy, i.e. water quality trading. The assembled watershed simulation system is further coupled with an economic analysis component, designed for simultaneously evaluating the environmental and financial performance of trading policies. The important factors (natural, environmental, economic and decision-related) and their associated uncertainties are carefully identified. Still employing the sampling-based RSA approach, the impacts of all these uncertainties on attainment of the dual targets of water quality trading are evaluated and those key constitsuents are identified. The framework and analysis of this chapter are shown to have an important bearing on decisions regarding appropriate trading ratio selection. This completes the demonstration of the overall framework for watershed management proposed in this dissertation.

Chapter 8 presents conclusions from the present research and makes recommendations on possible future lines of research.

Chapter 2

WATERSHED MANAGEMENT:

TMDL AND WATER QUALITY TRADING

2.1 Overview

Management of water resources is concerned with both water quantity and quality, and increasingly over recent years at the watershed scale. The management plan is usually harmonized by national or local authorities, aiming at improvements in both water resource conservation and pollution control. The relevant legislation in the United States has a long history. Since the beginning of the last century, the U.S. has enacted extensive federal legislation to fight water pollution. The Clean Water Act (CWA) of 1972 is the milestone piece of legislation for surface water quality protection (Field 2007). Under the requirements of the CWA, a number of watershed and water quality management policies have been developed and implemented for the purposes of water resource protection and water quality restoration.

However, in 2000, EPA conducted a comprehensive national survey of 33% of U.S. waters, finding that 40 percent of streams, 45 percent of lakes, and 50 percent of estuaries were failing to support their designated uses (EPA 2000a). There are more than 20,000 impaired water bodies throughout the United States, as shown in Figure 2-1. According to this survey, we may conclude that traditional regulatory approaches, which have been applied for 30 years since the 1970s, have only achieved inadequate results. Faced with these challenges, the government and stakeholders are seeking innovative, supplementary ways to achieve water quality goals.

TMDL and water quality trading, as two policy instruments, have therefore been introduced to overcome such difficulties. These two closely related policies are our focus in this dissertation. They are both frequently used at present, and recommended by EPA for further widespread implementation. Instead of a discussion of either sophisticated legislation or practical manipulation of the policies, this dissertation emphasizes the underlying technical methodology for providing a sound basis for effective management programs.

2.2 TMDL

2.2.1 A brief introduction

In the family of watershed management tools, TMDL is currently the most important and popular one for pollution control and protection of ambient surface water quality in the United States. It is not a new idea in environmental studies. In fact, it comes from the term "water environmental capacity", for which conceptual research and corresponding methodological developments for determining how much pollutant can be released while still maintaining the environmental attributes of the water, have been started in the 1970s. Deriving from this concept, the TMDL specifies the maximum amount of a pollutant that a waterbody can receive and still meet water quality standards, and allocates pollutant loadings among point and nonpoint pollutant sources (EPA 2008b).

Addressing the shortcoming of the NPDES (National Pollutant Discharge Elimination System), which is only for regulating the point sources that discharge pollutants into waters, the TMDL program is a planning tool for regulating both point and nonpoint sources, and is used to establish pollution budgets for polluted watersheds. It reflects shifting of the focus of water quality management back from effluent or source-based control to an ambient-based system. The EPA is strongly advocating it. In 2000, EPA issued very detailed regulations requiring that states determine the TMDL plans for each of their impaired waters.

The TMDL is believed to be an effective path for water quality management through a systematic and scientific approach. It includes three parts for calculation: waste load allocation for point sources (WLA), pollution load allocation for nonpoint sources and natural background conditions (LA), and a margin of safety (MOS) that accounts for the uncertainty that could undermine policy success. In developing a TMDL, first, the authority should enact the water quality standard based on the requirements of designated water use types (drinking, fishery, swimming or recreation). Then, the total allowable (critical) pollution load that enables the receiving water quality to be just equivalent to the standards is calculated. This is the maximum daily load that can by discharged into a water body.

In this process, the pollution-discharge/water-quality relation needs to be constructed based on a scientific/engineering analysis. Next, after investigation and evaluation of the sources that contribute to the stream or lake, the pollution load allocation is determined. Allocating the TMDL among different point sources and nonpoint sources means placing responsibility for emission reduction on sources. It requires the pollution source that fails to comply to take measures for achieving pollutant abatement, followed with enforcements (Harrison 2007). As a practical form of water environmental capacity, TMDL is actually more complicated than it seems. A TMDL program depends on extensive investigation and quantitative calculations regarding watershed hydraulic and pollutant properties, as well as a sufficient evaluation of the associated uncertainties.

During the past several decades, we have witnessed thousands of TMDL programs being established and implemented throughout the United States, addressing one or more constituents of sediment, pathogens, nutrients, metals, dissolved oxygen, temperature, pH, pesticides, mercury, and organics. According to U.S. EPA records, 33,903 TMDL programs have been approved since the year of 1995, and 3,515 of them concern the problem of nutrients (EPA 2008c).

2.2.2 TMDL modeling and uncertainties

Scientific research on TMDLs usually focuses on two interacting issues: modeling and uncertainties. Watershed models are recommended and extensively used for TMDL assessments, for evaluating the maximum pollutant discharges the water body can assimilate without water quality impairment, and predicting water quality in response to changes in pollutant loading and various allocation strategies. In the past several decades, hundreds of TMDL programs have been developed with the aid of watershed modeling tools in the United States and throughout the world (Borah et al. 2006; Chapra 2003; Lin and Radcliffe 2007; Munoz-Carpena et al. 2006; Neilson et al. 2002; Stow et al. 2003). However, we also notice that among all these case studies, there is still a lack of a universal and standardized paradigm, which is simple enough yet defensible to meet the technical demands of the TMDL program of quantitative computation and risk assessment.

The problem of the uncertainty involved is a major concern for those watershed management policies established based on TMDL calculations. Especially with the intensive application of large watershed models, it has been recognized that such models may have a large degree of uncertainty associated with their simulations. This uncertainty can significantly limit the utility of model output, for the uncertainty in the predictions of the TMDL and the efficacy of control actions could lead to the consequence that implementation actions might be ineffective and therefore wasteful of limited water quality resources (Shabman et al. 2007). Therefore, in 2001, the National Research Council (NRC) established a committee to examine the scientific basis of the US EPA's program. The overriding theme of the NRC report was that "…statements about the science behind water quality management programs must be made with acknowledgment of uncertainties" (NRC 2001). For TMDL programs, the NRC committee recommended more explicit evaluation and reporting of model prediction uncertainty in the development and implementation plans (Shabman et al. 2007).

Normally the problem of uncertainty in the TMDL is compensated for by the Margin Of Safety (MOS), which is set to a reasonable value reflecting a lowering of the pollution discharge permit below the calculated critical pollution discharge threshold. The MOS component in the TMDL is intended to account for uncertainty and risk, but currently it is often selected arbitrarily, as opposed to being based on a sufficient uncertainty analysis (Shirmohammadi et al. 2006). This will definitely impair the reliability and cost-effectiveness of TMDL assignments and derived policy. Therefore, in order to generate an effective and reliable TMDL plan, case studies are conducted for coping with the issue of uncertainty, especially in the process of modeling (Arabi et al. 2007;

Borsuk et al. 2003; Dilks and Freedman 2004; Neilson and Chapra 2003; Reckhow 2003; Reckhow et al. 2003; Wu et al. 2006).

Several studies conclude that more scientific approaches to account for uncertainty should be developed and applied. It has been proposed that explicit quantification of uncertainty be made an integral part of the TMDL process (Shirmohammadi et al. 2008). In this dissertation, we will accordingly construct a computational framework for calculating the TMDL based on modeling accompanied with an appropriate uncertainty analysis. Our ambition is that this method should become a standardized methodology for accounting for uncertainty in the TMDL and other watershed management policies.

2.3 Water quality trading

2.3.1 A brief introduction

With respect to the topic of watershed pollution control, it has recently been realized that only addressing control from the perspective of environmental engineering and technologies is far from sufficient. Economic and social issues are also considered as important paths to the management target. Since the 1990s, people have paid increasing attention to economic solutions for environmental problems. Among them, Water Quality Trading (WQT, and also known as watershed pollutant trading, or nutrient trading, if nutrients are concerned) is an innovative one which aims at making watershed pollution control cost-effective.

Given the fact that curtailing sources of pollution in a watershed can incur very different costs, even for the same pollutant, water quality trading allows 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, thus achieving the same water quality improvement in a more cost-effective manner (EPA 2008c). This approach provides a flexible method for pollution control. When the dischargers are required to make pollution reductions due to tighter effluent limits or when new pollution loads are produced, other than neutralizing it with a high economic cost, there is another option, to offset it. Where implemented properly, dual benefits from both environmental and economic perspectives will be generated. Trading has gained growing attention in both academic and practical contexts in past decades.

From the perspective of the economics of water quality trading, the permit for pollutant discharge is considered as a tradable commodity, since it bears the attribute of scarcity, exclusivity, transferability, and enforceability (Tietenberg 2004). The mechanism of the market is utilized for an efficient allocation of this environmental resource. After the initial discharge permit assignment, the policy of water quality trading allows permits to be transferred through the trading market, until arriving at a more economically efficient reallocation. Compared with the situation without trading, where each source has to control its pollution individually, this means a relatively lower total cost will be achieved through the functions of the market.

Water quality trading is practically related to TMDL programs. In many of the existing water quality trading programs, the TMDL is acting as the baseline or “cap” of the pollution load sources. It may yield realistic benefits under the condition that the TMDL plan imposes a pollution reduction requirement; when the total actual discharges in a watershed is somewhat higher than the assimilating capacity of waterbody, then water quality trading can be employed as a cost-effective tool for achieving the TMDL targets. Compared with the relatively straightforward concept of the TMDL, the subject of water quality trading seems much more complex. We will therefore further introduce the conceptual basis and essential features of WQT in the following paragraphs.

The concept of pollutant trading originated in the field of air quality as emissions trading (Tietenberg 1985). The early applications include a trading of sulfur dioxide and nitrogen oxides for acid rain control and carbon dioxide in the international burden-sharing acts under the Kyoto Protocol. During the past two decades, mature markets have already been set up for atmospheric emission trading throughout the world and emission trading has become a rather regular policy for air-pollution management. Compared with the atmospheric emission trading programs, watershed pollutant trading is younger, and has greater potential.

EPA's policy endorses the use of water quality trading for certain pollutants as an economic incentive for voluntary pollutant reductions and as a way to achieve the Clean Water Act goals. They believe that this kind of market-based approach can provide greater flexibility, with potential to achieve greater water quality and environmental benefits, at least, greater than would otherwise be achieved under more traditional regulatory approaches. More specifically, the practical benefits of water quality trading may include the following aspects: 1) establishing economic incentives for voluntary pollutant reductions from point and nonpoint sources within a watershed; 2) reducing the cost of compliance with water quality objectives and reductions established by a TMDL; 3) offsetting new or increased discharges resulting from growth in order to maintain levels of water quality that support all designated uses; 4) providing the means to manage growth while protecting the environment; 5) achieving greater environmental benefits than those under existing regulatory programs; 6) providing substantial incentives for stakeholders to control unregulated nonpoint source pollution; 7) encouraging further adoption of pollutant prevention and innovative technologies; 8) securing long-term enhancement in water quality through the purchase and retirement of credits by any entity (EPA 2003).

Environmental policies can be principally classified into three categories: command and control, economic incentives, and a mixture. In the past much of pollution control management has been focused on compliance with "end of pipe" standards, requiring dependence on the command and control system. As an economic solution for internalizing the externality of pollutants, the market-based approach is often considered to be cost-effective compared to the command-and-control approach of traditional environmental regulation (Msangi et al. 2005; Tietenberg 2004). Water quality trading is a specific representative approach in the group of transferable permit schemes (Harris 2006; Tietenberg 2006). Compared with the traditional command-and-control (regulatory) system and the widely used other economic approaches (Horan and Shortle 2001), water quality trading can be regarded as a combination of regulation (under the mandated discharge cap, which is often set by the CWA) and economic stimulation. From a comparison among these tools, listed in Table 2-1, we see that water quality trading has advantages over the traditional command and control or other economic policies, yet requires more effort in its development and manipulation.

All the watershed pollution control tools listed in Table 2-1 are economic approaches except the first column. TMDL programs are often proposed for generating an appropriate permit for pollution sources, and can be considered as an auxiliary tool for regulating the pollutant discharge.

Water quality trading is a cost-effective approach to achieving compliance with ambient standards, but it is imposed on sources, so there is a "both" in the corresponding element of Table 2-1, i.e. for both "Source and Ambient-based".

2.3.2 Water quality trading programs

The EPA enthusiastically supports both the concept and implementation of water quality trading. In January 2003, EPA issued its Water Quality Trading Policy to provide guidance and encouragement to develop trading programs (EPA 2003). This policy has greatly advanced water quality trading by further enabling and supporting the adoption of market-based programs for improving water quality. Water quality trading has been attracting great interest and we see many pilot projects have been proposed and implemented throughout the world. These programs are supposed to save millions of dollars while significantly reducing the amount of water pollution. The nation's first watershed pollutant trading program was established for the Dillon Reservoir in Colorado in 1984 (EPA 1996). At present, over twenty states are in various stages of developing over one hundred trading programs (Breetz et al. 2004). Figure 2-2 shows the location of water quality programs in the U.S. at different stages (Morgan and Wolverton 2005).

Elsewhere, outside the U.S., water quality trading has also been proposed for applications in Canada, Australia and Europe (Sauvé et al. 2006). In China, the concept of water quality trading is discussed mainly as discharge permit trading. Several pilot trading programs are conducted in Nantong City, Jiangsu Province, as a point-point trade between public wastewater treatment facilities and industrial factories, and Lake Tai, as a point-nonpoint trade for controling pollution loads from paddy lands or other agricultural areas (Luo et al. 2005; Wang et al. 2004). In Georgia, water quality trading has recently started to attract some attention. Some essential research has examined the feasibility of potential applications (Rowles 2005; Rowles et al. 2006). Another project in Georgia has also been conducted to study the potential use of phosphorus-credits trading in the watershed of Lake Allatoona (Radcliffe et al. 2003; Radcliffe et al. 2007).

Although there is not much direct evidence of the successes or failures in actual practice of pollutant trading, observation of the existing trading programs still indicates that trading has the potential to improve water quality in heavily impaired watersheds (McGinnis 2001) and to yield great economic benefits (WERF 2000). An EPA survey shows tremendous financial benefits can be achieved when adopting water quality trading to achieve more cost-effective implementation of TMDL programs. This survey has examined costs to implement 36,000 TMDLs for 20,000 impaired waters in U.S., and estimated that application of flexible approaches (with a cost of $900 million to $3.2 billion) could save at least $900 million dollars annually compared to the least flexible approach (with a cost between $1.9 billion to $4.3 billion) (EPA 2001b). Another example in China shows that potential trades for chemical oxygen demand discharges achieve an annual cost-saving of 18.4% of the total annual cost of attaining the reduction target without trading (Tao et al. 2000).

In practice, for current watershed pollutant trading programs in the U.S., we see that the system of “baseline and credit” is usually implemented (Nishizawa 2003). Under this system, the permissible baseline discharge level set by the government should be at or below the current discharge level. This means that when a source maintains the baseline and reduces its amount of discharge, this is called a “credit”, which is the equivalent of the baseline minus the actual discharge level. This credit amounts to a permit, which, if unused, can then be sold. The discharger obtains credits only if and when it reduces pollutant discharge. Therefore, the baseline and credit system will not lead to an increase in the total discharge level. The U.S. EPA is highly recommending this system as a standard form for pollutant allocation trading, and most of the programs currently in operation are of this type.

The programs of water quality trading can have various forms, such as volunteer credit trade between stakeholders, transactions under the supervision of an environmental authority, or a government-manipulated credit bank, which purchases surplus pollution credits and sells them to those who need extra discharge permits. This last is normally believed to be better considering the issue of operational feasibility and reliability. In addition, the watershed total pollution discharge can conveniently be managed through the adjustment of credits held by the credit bank, quite similar to the functions of banks to intervene in the economy. For example, if we want to improve water quality by tightening watershed discharge permits, the bank may be asked to conserve (or buy, if the deposited credit is zero) a certain amount of credits. It is a very typical and good example of environmental management through economic methods.

2.3.3 The problem of uncertainty

The uncertainty associated with water quality trading is more significant, for there is not only uncertainty in the application of environmental models, but also risk and uncertainty in market behavior and economic analysis (Wesseler et al. 2003). However, most of the past research on uncertainty has been confined to the evaluations of pollution sources. Many cases focus on examining watershed conditions and estimation of the point and nonpoint sources to assess the feasibility of a policy in a particular watershed (Obropta 2004; Obropta and Rusciano 2006; Rowles 2005). Meanwhile, we have also noticed that some research has conducted efforts in using watershed models to evaluate watershed pollutant discharges for developing water quality trading programs. For example, a stochastic programming model and a combined probabilistic simulation are employed to assess the feasibility and cost-effectiveness of point-nonpoint sources effluent trading in the Lake Tai watershed, China (Wang et al. 2004). In another study of the same watershed, considering the main uncertainty sources as a stochastic, interval, and fuzzy format, a model has been developed to quantify the efficiency of potential trading efforts (Luo et al. 2005). In the Chesapeake Bay Nutrient Trading Program, the HSPF model has been applied for calculation of nutrient and sediment loadings and nutrient removal efficiencies of nonpoint BMPs (Best Management Practices), hence to provide information for trading scheme determination (Wiedeman and Trask 2001). In the program of Lake Allatoona, in conjunction with the application of the SWAT model, a software named PEST has been employed to assess the involved uncertainties (Radcliffe et al. 2003; Radcliffe et al. 2007).

Where designed and implemented appropriately, water quality trading can be a powerful tool for the improvement of financial profits, as well as environmental and ecological benefits, but it has various obstacles as well. In fact, only a small portion of the water quality trading programs have achieved outcomes as expected, due to various reasons (Breetz et al. 2005). There are many documented unsuccessful water quality trading programs, caused by types of market failures or limitations, such as low market supply and demand, over or insufficient regulation (King and Kuch 2003), information access barrier, manipulation problem and non-rational behavior (reluctance for participation). Besides these practical reasons, from the technical perspective, an important obstacle that hampers wider adoption is the lack of a systematic approach for analyzing the associated uncertainties. Since significant uncertainties are involved in the estimation of pollutant sources, their transport and fate, performance of pollution control practices, prediction of post-trading water quality, cost assessments, and future development scenarios, trading schemes should be assessed with a clear account of the consequences of all such uncertainties. In order to make water quality trading programs both credible and successful, the issue of uncertainty should be fully addressed and quantitatively accounted for, by means of a comprehensive and reliable uncertainty analysis process (Boyd et al. 2004; Chakraborty et al. 2004; EPA 2003).

A number of approaches have been suggested to compensate for the uncertainty in water quality trading. Among them, the trading ratio method is the most important one (Hung and Shaw 2005). Its role in the context of water quality trading is similar to that of the MOS in TMDL programs. The trading ratio specifies the rate at which nonpoint source (NPS) abatement can be substituted for point source (PS) abatement. This implies the following: given an amount of pollutant abatement, determine how much credit (to pollute elsewhere) can be sold so that the resulting stream water quality is at least as good as the condition before trading happens. A trading ratio of NPS:PS>1 is often used, particularly for those relatively conservative pollutants such as total phosphorus, given the sense that the credit a pollution abatement practice (by nonpoint sources) can generate and sell (usually to point sources, who face higher control costs) should be less than the quantity of the reduction. The purpose of the trading ratio is to prevent the risk of possible environmental impairment due to the offset and the relocation of pollution. Consequently, one important quantitative task in designing the pollutant trading scheme is to evaluate the transport of pollutants among different dischargers for achieving the so-called water quality equivalence.

Multiple methods are used to determine the trading ratios. Some employ a simple conservative estimation method, and in more cases we see the application of mathematical models to determine the value of the trading ratio. For example, some research suggests using a geographic information system (GIS) and the finite segment method to consider the decay of pollutant and estimate the appropriate values of the trading ratio (Curley 2003). Other programs compartmentalize the trading ratios into Delivery Ratios (Location Ratios), Uncertainty Ratios (Uncertainty Discount), Water Quality Ratios (Special Needs Ratios), and Retirement Ratios (O'Grady and Wilson 2000; Wiedeman and Trask 2001). In particular, in a significant study for exploring water quality trading under uncertainty, the optimal trading ratio is evaluated based on the simulation of water quality equivalence of pollutant reductions at different discharge sources (Shi and Beck 2007b).

We consider that the research into uncertainty for water quality trading is curretly rather deficient. The topic should be studied in depth and expressly for the requirements of scientific watershed management. In most research, interests are confined to nonpoint-source estimation, such as varied rainfall and pollutant yield; no one is bothering to analyze uncertainty in respect of point-source discharges or the economic issues. There is no comprehensive and integrated framework method for evaluating water quality trading with comprehensive and clear consideration of the inherent uncertainties. This is also a common challenge for many such type of issue at the interface between science and policy. To that end, this dissertation and some preliminary research (Shi and Beck 2007a; Shi and Beck 2007b) have attempted to set up a systematic and scientific methodology for handling and quantifying uncertainties from a variety of sources and their impacts on the predicted performance of trading programs.

Table 2-1: A comparison among watershed pollution control tools

	Command & control	Emission tax	Input or output tax	Environ. subsidies	Nutrients trading
Cost effectiveness	Low	High	Medium	Low	Medium
Environmental benefit	High	Medium	Medium	Medium	High
NPS Monitoring required?	Yes	Yes	No	No	Yes
Information Required	Low	High	Low	Low	High
Transaction cost	Low	High	Medium	Low	High
Administration/Enforcement	Medium	Hard	Easy	Easy	Hard
Source or Ambient-based?	Ambient	Source	Source	Source	Both
Institutional requirements	Low	Medium	Medium	Low	High
Flexibility	Low	Medium	Medium	High	High
Overall complexity	Low	High	Medium	Low	high

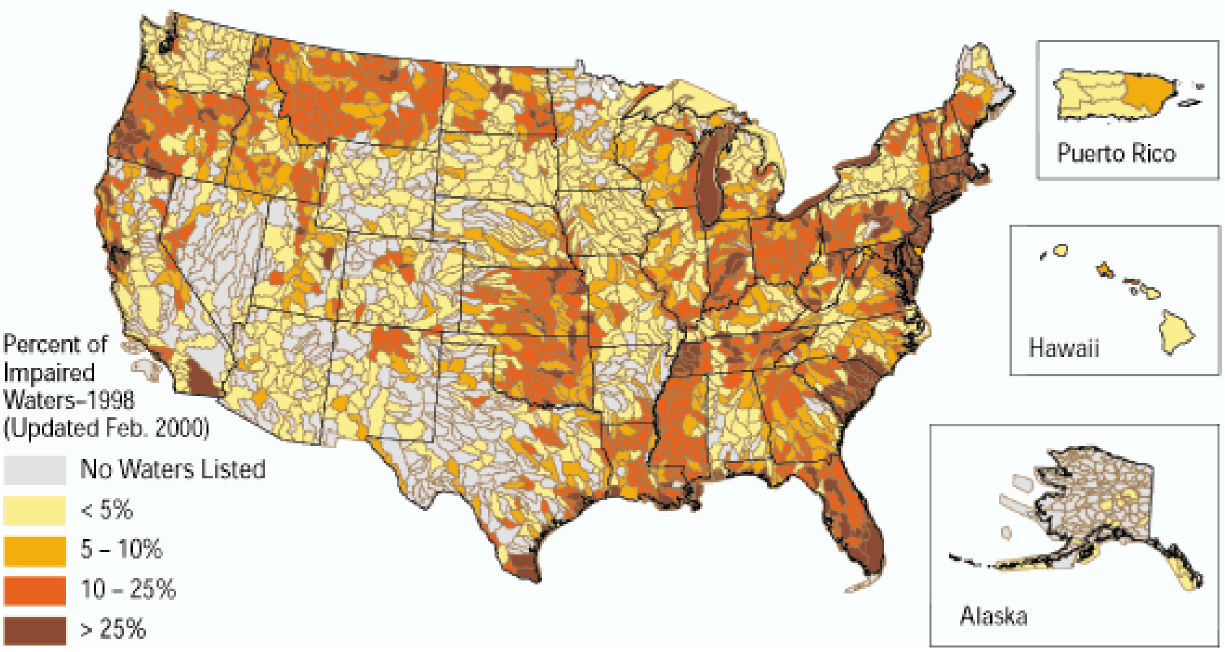


Figure 2-1: Map of watersheds containing impaired water bodies

(EPA 2000a)

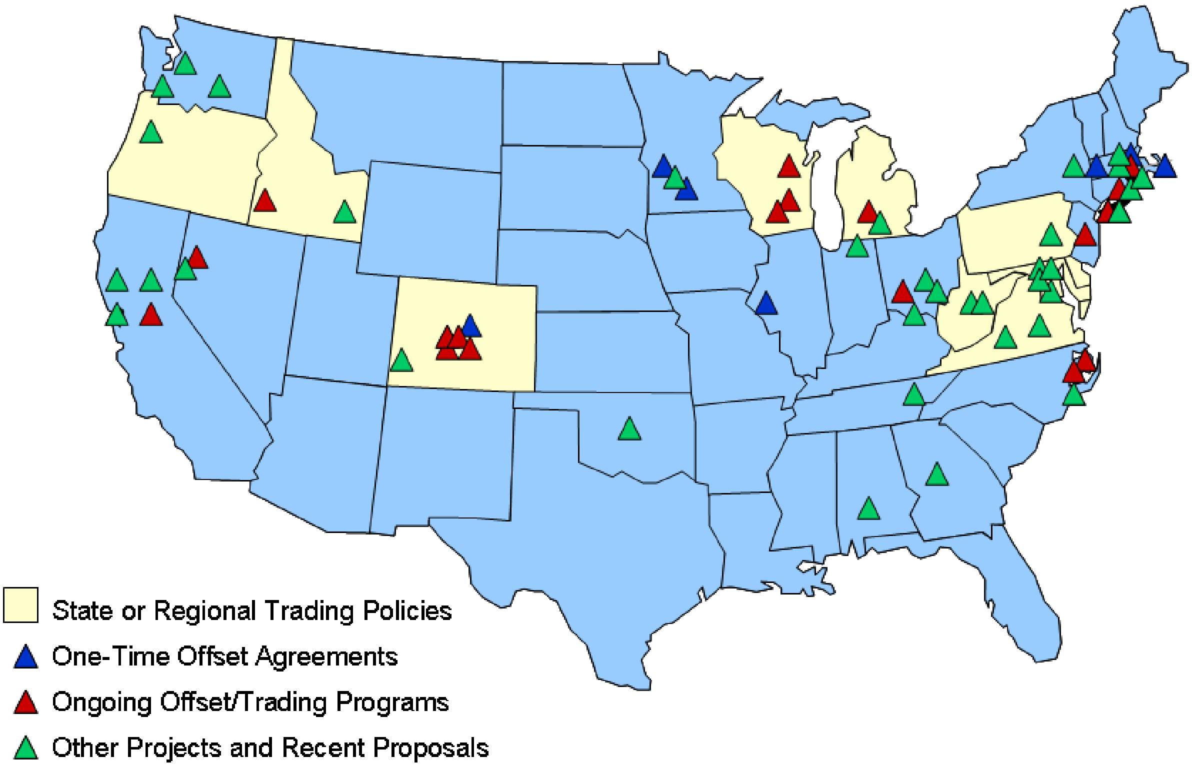


Figure 2-2: Water quality trading programs in U.S.

(Morgan and Wolverton 2005)

Chapter 3

A REVIEW OF WATERSHED MODELING AND UNCERTAINTY

3.1 Watershed and water quality modeling

3.1.1 Modeling in environmental study

Models express our understanding of the behavior of a real system with mathematical relationships. The aim of modeling is to evaluate whether the effect and outcomes we have observed are reproducible from the current knowledge of unobserved or underlying processes (Wainwright and Mulligan 2004). In the current era, modeling has become an important path for advancement of the sciences (Kirchner 2006). This trend is even more notable in the field of environmental research. Environmental models are used to reveal and describe the internal mechanisms of the given environmental system; provide quantitative enumeration of the incorporated state variables and their responses to influential factors, for example, the change of climate or disturbance of human activities. In addition, a higher goal of modeling is predicting the future, under conditions radically different from those observed and discovered in the past (Beck 2002; Beck 2005a). In concert with the changes in natural and societal systems, modeling provides a robust path for extrapolating to future conditions based on current knowledge.

In environmental system analysis, and the new field of environmental informatics, mathematical models can be seen as a core component. They interpret the data obtained by monitoring, simulate the system behavior, and provide quantitative assessment and scientific support for associated environmental planning and management. Figure 3-1 gives an illustration of such a context. The framework shown here can be considered as conventional for environmental system analysis, and the research for this dissertation will follow this general scheme, incorporating all these components and exploring the interactions between them.

More specifically, for a management-oriented research driven by the task of supporting the decision-making process, models play an important role. The procedures of a modeling-based environmental decision-support system are shown in the flow chart of Figure 3-2, in which models are employed principally to estimate the consequence of a given management policy, for evaluating the efficacy, for screening out the “good” policy, or for implementing strategies. As far as the present study is concerned, models constitute the scientific basis for the entire framework. Working with a dynamic watershed simulation tool, the systematic framework of modeling under uncertainty for supporting environmental management is constructed and applied in this dissertation.

3.1.2 Watershed modeling

Today in watershed-scale research, hydrologic and water-quality models are extensively used to help investigate and understand complex watershed processes. Watershed models have become an important tool in addressing a wide spectrum of environmental and water resource problems including water resource planning, development, design, operation and management (Singh and Frevert 2006). Watershed models simulate the mechanisms of the flow of water, sediment, chemicals, nutrients, and ecological processes, and predict receiving water response to changes in environmental, natural and social, impacts, They are used as links between sources of pollutants and the receiving water. From a summary of popular watershed models (Singh and Frevert 2006), we see that dozens of watershed models have been developed and applied for watershed research. In addition, the flourishing of watershed modeling in the late 20th century has been to some extent stimulated by the recognition that nonpoint source pollution dominates many water quality and ecological problems, in particular, since nonpoint discharges are hard to monitor directly and thus require estimation with watershed models.

Since the appearance of the Stanford Watershed Model in the 1960s, watershed modeling has arrived at a broad consensus that mechanistic models are definitely superior to the earlier empirical models. Over the decades, there has been a trend for modeling tools to evolve from simple statistical models to spatially-explicit, process-based, dynamic models. Environmental modeling studies have always been focused on the development of models with ever more complicated structure, incorporating more processes and parameters, in order to mimic the natural system in as many specific details as possible.

While discussing the topic of mechanistic models, we cannot ignore the long-lasting debate on the topic of simplicity and complexity in environmental modeling (Young et al. 1996). The main advantage of high-complexity models is that they (try to) simulate the complex system mechanism on a more detailed physical basis. Ideally, as long as we could build the models totally based on the Laws of Physics, we could make a perfect extrapolation beyond the trend that has been observed in the past. However, this is not yet achieved in current environmental model studies, which contain a large complexity not described with a "firm" physical theory. In principle, all the current environmental models, contain parameters whose values will have to be assigned based on attempts at reconciling the performance of the model with observation of the in situ system behavior. In other words, they are all subjected to the process of calibration, or so-called "data-based". Because of the parametric equifinality, different parameter (vectors) will probably result in the same model outputs or same extent of fitness to the observations, so the calibration process is often unable to get good estimation for some parameters. In other words, these models will be to some extent unidentifiable. Some, however, believes that typical rainfall-runoff data only contain enough information to constrain 4 parameters (Jakeman and Hornberger 1993). By this reference, most of the current hydrological models are over-parameterized. In many cases, the crux of the problem of a lack of model identifiability, or over-parameterization, is that what one would like to know about the internal description of the system is of a substantially higher order than that which can be observed of its external description (Beck 2002).

The problem of over-parameterization will definitely bring extra difficulties and hamper the effectiveness of model identification and the reliability of the subsequent prediction process. Therefore, it is important to choose an appropriate complexity during model development. Dr. Einstein said, "The process should be described simply, but not too simply." The optimal model is one that contains sufficient complexity to explain phenomena, but no more (Wainwright and Mulligan 2004). Thus we suggest that in a watershed study, a solution might be, to choose parameters which have a definite physical meaning and whose confident values are easily obtained from experiments, while for those parameters that can only be obtained by calibration, limit their number to as few as possible. In addition, the power of models lies in the way they are applied, not in their dimension or conceptual complexity.

3.1.3 Examples of watershed models

In the family of physically-based watershed models, SWAT (Soil and Water Assessment Tool) (Arnold et al. 1998) and HSPF (Hydrologic Simulation Program-FORTRAN) (Bicknell et al. 2005), both embedded in the BASINS system (EPA 2001a), are considered as the two most popular in the United States. Another distinctive model that attracts considerable interest is AGNPS (AGricultural Non-Point Source pollution model) (Young et al. 1994), which is featured with a fully distributed model structure. The present research also relies heavily on a recently developed model named STAND (Sediment-Transport-Associated Nutrient Dynamics) (Zeng 2001), for addressing dynamic river water quality issues. Consequently, we will briefly summarize the primary features of these models, in order to obtain a general sense of the state of the art of watershed modeling, and gain helpful illuminations for subsequent research in watershed simulation and assessment.

(1) SWAT

SWAT is a conceptual, continuous-time model that was developed in the early 1990s to assist water resource managers in assessing the impact of management policies and climate variability on water supplies and non-point source pollution in watersheds and large river basins. In SWAT a watershed is divided into multiple sub-watersheds, which are then further subdivided into hydrologic response units (HRUs) that consist of homogeneous land use, management, and soil characteristics. SWAT has a semi-distributed spatial structure, due to the fact that it is parameterized into the HRU level (each HRU has its own parameter sets).

The model has an upland component which includes weather, hydrology, erosion/sedimentation, soil temperature, plant growth, nutrients, pesticides, agricultural management, together with stream routing and pond/reservoir routing components. The upland component generates the daily discharge, sediment and pollutant load throughout every HRU in the watershed. It has also a stream component, which includes channel flood routing, channel sediment routing, and nutrient and pesticide routing and transformation. Additionally, the pond and reservoir component contains water balance, routing, sediment settling, and simplified nutrient and pesticide transformation routines.

The hydrologic processes simulated in SWAT include: surface runoff estimated using the SCS (U.S. Soil Conservation Service) curve number or the Green–Ampt infiltration equation; percolation is modeled with a layered storage routing technique combined with a crack flow model; lateral subsurface flow; groundwater flow to streams from shallow aquifers; potential evapotranspiration by the Hargreaves, Priestley–Taylor and Penman–Monteith methods; snowmelt; transmission losses from streams; and water storage and losses from ponds (Arnold and Fohrer 2005; Arnold et al. 1998). HRU-level and in-stream pollutant behavior can be estimated for sediment, nitrogen, phosphorus, pesticides, and bacteria. Sediment yield is calculated with the Modified Universal Soil Loss Equation (MUSLE) (Williams and Berndt 1977).

The transformation and movement of nitrogen and phosphorus within an HRU are simulated in SWAT as a function of nutrient cycles consisting of several inorganic and organic pools. More specifically. the soil phosphorus is assumed to be comprised of three pools, inorganic (approximately soluble mineral phosphate), active and stable organic (mostly the insoluble particulate form). The soil phosphorus processes in the model account for decay of plant residue, decomposition of the fresh organic matter, mineralization and immobilization, adsorption and desorption, and plant uptake. The amount of soluble phosphorus removed in runoff is predicted using soluble phosphorus at the top soil layer, the runoff volume and a partition factor. Phosphorus transported with sediments is calculated by a loading function which estimates the daily organic phosphorus runoff loss based on the concentration of organic and active inorganic phosphorus in the top layer, the sediment yield, and an enrichment factor (Gassman et al. 2007; Nasr and Bruen 2003).

(2) HSPF

HSPF is an EPA computer model for simulation of watershed hydrology and associated water quality for both conventional and toxic organic pollutants on pervious and impervious land surfaces and in streams and well-mixed impoundments. Since its initial development nearly thirty years ago, the HSPF model has been applied throughout North America and numerous countries around the world. The HSPF model incorporates the watershed-scale Agricultural Runoff Model (ARM), Non-Point Source models, and pollutant transport models, into a basin-scale analysis framework.

It uses information such as the time series of rainfall, temperature and solar radiation, land surface characteristics such as land-use patterns, and land management practices, to simulate the processes that occur in a watershed. The result of this simulation is a time series of the runoff flow rate, sediment load, and nutrient and pesticide concentrations, along with a time series of water quantity and quality at some points in a watershed. Its hydrological component for the land phase includes three flow types: surface runoff, interflow, and groundwater discharge, the portions of which are determined by processes of infiltration, loss to deeper groundwater, and storage in the upper and lower soil layers. Channel hydraulics are calculated primarily based on the depth-flow relationship expressed by a so-called F-table. HSPF simulates three sediment types (sand, silt, and clay), in addition to a single organic chemical and transformation products of that chemical. Regarding nutrient pollutants, HSPF can be used to simulate nitrogen, as the forms of ammonia (NH_3 and NH_4^+), nitrite, nitrate, and phosphorus, as the form of orthophosphate. Despite the complicated description and flow chart of this model, especially for the pollutant simulations, it actually employs rather straightforward methods. Specifically, in the pollutant simulation component (named PQual and IQual), the pollutants are considered as associated with either flow or sediment, or both. Accordingly, the flow-associated pollutant behavior is described by accumulation and storage limit parameters, and the sediment associated pollutant release is determined by the parameters of washoff and scour potency factor.

HSPF is widely recognized as the most comprehensive and scientifically defensible process-based model of watershed hydrology and water quality that allows the integrated simulation of land and soil contaminant runoff processes with in-stream hydraulic and sediment-chemical interactions.

(3) AGNPS

AGNPS, developed by USDA (United States Department of Agriculture) Agricultural Research Service (ARS) scientists and engineers, is an event-based model that simulates essentially the rainfall-induced surface runoff, sediment, and nutrient and pesticide contributions from overland flow to streams, primarily from agricultural watersheds. Since it was originally published in the late 1980’s, it has been widely used to provide estimates of runoff water quality and non-point pollution yield, and to quantify the effect of management decisions on a watershed system in many regions all over the world. The unique feature of AGNPS is that it has a fully distributed model structure, which is achieved by subdividing the watershed into gridded square elemental areas, and each cell is assumed to have uniform physical characteristics and has identical parameter values. The hydraulic and pollutant behavior of each cell is evaluated by a plot-scale simulation unit. The model routes the physical and chemical constituents from each cell into the stream network and finally to the watershed outlet.

The model operates on a cell basis, which makes it possible to analyze spatially discrete management units within a watershed, thereby enabling identification of the sources of the pollutants at their origin and tracking them as they move through the watershed system, thus to focus on critical source areas of nutrient export (Young et al. 1995). Compared with semi-distributed watershed models, such as SWAT and HSPF, which work at the level of an HRU (in the same subbasin, with the same land-use type and soil property), the model of AGNPS bears a better description for the watershed hydraulic processes. The advantage of this model is demonstrated in many valuable previous studies. For example, AGNPS has been applied to predict nonpoint pollution yield from intensive agricultural areas in Dianchi basins (Shi et al. 2005), and has been incorporated in the decision support system for aiding practical watershed planning and water quality management of the Guanting reservoir (Shi 2002).

Since its original construction on a single-event basis, many enhancements have been realized to improve its capability. For example, the incorporation of CCHE1D for stream networks and

CONCEPTS for stream corridors include more detailed science for the channel hydraulics, morphology, and transport of sediments and contaminants. More significantly, AGNPS was recently superceded by an annualized continuous-simulation version (AnnAGNPS), which combines the latest advances in GIS data manipulation and physical characterization of the catchments and operates with a daily time-step, designed to simulate long-term (as opposite to sing-event) chemical and sediment movement, for providing more powerful support for watershed planning and management (Bingner and Theurer 2005).

(4) STAND

The STAND model is an advanced stream hydrological and water quality model developed at the University of Georgia. It was originally developed to address the water quality issues associated with sediment behavior in streams and rivers under transient hydraulic conditions (and tailored to conditions typical of the Piedmont region). While addressing water quality issues, STAND simulates channel flow, sediment transport and interactions with other water contaminants.

It has a three-level structure: the base level contains the hydraulic component, which uses the conventional de St Venant equations to compute one-dimensional open-channel hydraulics and provide information to the higher levels of the model for further computation. The second level is the sediment transport level. Sediment transport potentials and actual sediment transport rates (of sand, silt, and clay size groups) are computed and provided to the top level, and the river morphological change is simulated as well. The water quality component is at the third level, the top level of the model. Here orthophosphate, nitrate, ammonium, and dissolved oxygen are simulated, and variations of their concentrations along the studied river are computed as a function of nutrient transport, adsorption/desorption of nutrients to suspended sediment, and releases from bed-sediment pore water. STAND employs thirty parameters and a set of partial differential equations to characterize the instream fluvial processes. The equations are solved by means of numerical integration, with a standard Preissmann Scheme.

STAND has been evaluated against a comprehensive data set obtained from a section of the Wei River, a major tributary of the Yellow River, in China, and sediment and nutrient data from the Oconee River, Georgia, a Piedmont river similar to the Chattahoochee (Zeng and Beck 2001; Zeng and Beck 2003). Compared with the other existing river models, it is essentially well suited to simulate streams in which transient sediment behavior is of central concern.

3.1.4 Improving watershed modeling

From the above review of watershed hydrologic and water quality models, we see that a number of critical issues have been addressed by modelers, especially for the purpose of enabling watershed modeling as a powerful tool to be employed for tasks of management support. The state-of-the-art of watershed modeling research depends on many factors such as management concerns, environmental assessment techniques and criteria, scientific knowledge of hydrologic and water quality processes, and availability of technology and data (Chen 2004). According to our understanding and experiences in model development and application, improvements can be further suggested as follow. These too will be addressed throughout this dissertation.

(1) Improving monitoring

Juxtaposed with the topic of modeling, environmental monitoring or data collecting is another important component in environmental systems analysis. Data are the foundation of any modeling effort. The criteria for assessing a model are not anything but whether it can appropriately reflect the real-world system behavior, and this is normally expressed by fitting model outputs with the observations. Observations of the modeled system are a vital prerequisite for model verification and analysis. In fact, at present, data quality often behaves as the bottleneck of many research exercises in environmental modeling. And what is more, an important reason for the over-parameterization of widely-used models, such as SWAT and HSPF, is that only deficient observations are available relative to the complexity of the model.

(2) Integration with advanced computer techniques

Rapid advances in computer technology have offered tremendous opportunities and potential for modelers to develop and manipulate the new generation of watershed models. These changes have dramatically increased computational efficiency, and enabled the application of numerical algorithms. Another recent revolution is that the development of various user-friendly, Windows-based interfaces makes model operation much easier. More significantly, the revolution of information technology, such as database and web-based techniques, has tremendously increased the function in data storage, organization, sharing, and analyzing. And the techniques of GIS (Geographical Information System) and RS (Remote Sensing) have enabled the convenient collecting and processing of geographical information, thereby opening up the new field of spatially distributed modeling.

(3) Advancement of computational algorithms

Computational algorithms are the “heart” or “engine” of watershed modeling. Most of the widely applied models were developed in the 1970s and 1980s, before the current generation of computers and technologies emerged and rapidly advanced. With the emergence of new computer techniques, computational algorithms should be refined for better utilizing the huge amounts of information and availability of high-speed computers. Fortunately, we see that a number of new algorithms, such as neural networks, evolutionary algorithm or generic algorithms, and distributed computation are emerging, being intensively explored, and employed in environmental modeling. The development of computational algorithms will continue to be an important direction of the relevant scientific advancement. In particular, as far as the watershed models are concerned, the advancement of computational capacities enable models to be designed and adapted at a rather high frequency, which is especially helpful for simulating the dynamic features of watershed hydraulic and nutrient behavior.

(4) Uncertainty analysis

Due to the inherent uncertainty associated with model applications, the uncertainty should be fully addressed and quantitatively accounted for to ensure the quality of modeling. This point will be discussed in more details in Section 3.2.

(5) Environomental management

The target of decision-support modeling is to serve as a scientific basis for solving real-world environmental problems. In fact, dynamic watershed models at present are playing a rather limited role for providing substantial support for planning and management issues. Further research is required for translating the modeling results into robust environmental policy. For this purpose, focusing on watershed models, various types of decision support system (DSS) (Du et al. 2003; Shi et al. 2005) have been developed as powerful and beneficial tools, in principle, for providing applicable interpretation of model results. DSS is to assist us in evaluating different management policies in a more efficient and user-responsive way. Additionally, based on the perception that policy making and planning processes require ongoing active engagement and collaboration between stakeholders, scientists and decision makers, the term of "participatory modeling" has recently been coined for incorporating stakeholders into the modeling process to support decisions involving complex natural resources questions (Voinova and Gaddis 2008). More involvement of stakeholders and interactive functions is thus another new feature of watershed models.

3.2 Analyzing uncertainty

3.2.1 Uncertainties in environmental modeling

Uncertainty has become a focal point in environmental research over the past couple of decades. An environmental system is a complex assemblage of interacting physical, chemical and biological processes, which are normally highly nonlinear and dynamic, with considerable uncertainty about both their nature and their interconnections (Young et al. 1996). Uncertainty is therefore an inherent attribute. Uncertainty and its influence in the identification and application of mathematical models is required to be explored to assure the quality, or the trustworthiness, of a model's performance (Beck 1987; Beck 1994; Beck 2002). Accounting for uncertainty in models is one of the so-called "grand challenges" of environmental modeling (Beck et al. 2008a).

A systematic uncertainty analysis process is an indispensable component of environmental study (Gabbert and Kroeze 2003; Zheng and Keller 2007). In particular, when we are facing the task of developing environmental policy based on our understanding of the environmental system, and due to the involvement of both social and economic issues, the amount of uncertainty is especially large. For interdisciplinary problems of environmental management, studies in risk analysis are especially necessary for supporting the making of decisions under uncertainty (Jordaan 2005). Therefore, an analysis intended to provide insight into the behavior of a system has to provide an assessment of uncertainty and its influence on the subsequent decision-making phase.

In watershed studies, substantial uncertainty exists in the model structure, its parameters and the associated field measurements. Such problems are further compounded by inadequate observations, in particular, the difficult and expensive task of monitoring transient events, and the relatively insecure science base of the generation and transport of runoff-induced sediment and sediment-tied and biologically transformed nutrients, such as phosphorus. These have resulted in significant uncertainties in predicting the impacts of watershed pollutant loads on the receiving water quality, thereby increasing the risks of failure at a subsequent decision stage, for the task of model-supported environmental planning and management. Nowadays, uncertainty assessment is an indispensable accessory to be added after the completion of modeling work.

3.2.2 Sources of uncertainties

Analyses of the behavior of complex systems typically involve two types of uncertainty: aleatory and epistemic (Helton 1994; Helton and Burmaster 1996). The definitions are based on the origins of the uncertainty, respectively: from what is considered an inherent randomness in the behavior of the system under study, or from a lack of knowledge about the value of a quantity in the context of a particular analysis. In environmental modeling, aleatory uncertainty derives from the system stochasticity and variability, while epistemic uncertainty can be categorized into two forms: limits on the data availability and on conceptual understanding of complex systems. Specifically, there are several notable studies on classifying sources of uncertainty in environmental modeling from different perspectives (Beck 1987; Beven 2008; Krupnick et al. 2006; Morgan and Henrion 1990; Piegorsch and Bailer 2005; Van Asselt and Rotmans 2002). These contributes have similarities in expressing the major sources of modeling uncertainty as: data scarcity or error in measurements, uncertainty in model structure, parameterization, stochasticity and variability in the natural world. Furthermore, when a model is applied for decision support, more uncertainties will be involved, such as uncertainties in scenarios (possible future state), inaccurate translation of model outcomes into policies, possible policy ineffectiveness, risk of improper and discontinuous implementation, and lack of enforcements. Compared with extensive studies on models, explorations of decision-stage uncertainties are less advanced.

More significantly, in a rather comprehensive review of the analysis of uncertainty for water quality modeling, Beck stated that four areas are associated with uncertainty in water quality mathematical models (Beck 1987): 1) uncertainty about the relationships among the variables characterizing the dynamic behavior of systems, which is uncertainty about model structure, 2) uncertainty about the value of the parameters appearing in the identified structure of the model for the system's behavior, 3) uncertainty associated with predictions of the future behavior of the system, and 4) the design of experiments, or monitoring programs, for the specific purpose of reducing the critical uncertainties associated with a model. Based on these discussions and our prior experiences on environmental modeling studies, in this dissertation the sources of uncertainties are evaluated according to the four categories set out below.

(1) Model structure

As a problem in hydrology and environmental systems analysis, structural uncertainty is now attracting increasing attention (Beven 2005). Complexity is the inherent attribute of an environmental system. Because the development of even the most advanced physically-based environmental models is still a simplification or abstraction of the complicated real-world system, uncertainties are inevitably introduced when we construct the model with mathematical equations. Figure 3-3 schematically illustrates such a process. We have spent forty years to build complex models to push the mathematical form approaching that of the real natural system; however, at least for contemporary watershed modeling, research shows that even the most complex model structure adopted is quite inadequate compared to the processes in real world.

(2) Parameterization

When we face the problem of determining parameter values, in most cases we cannot assess the "true value", otherwise the parameter would be replaced by a "constant". Parameters must be calibrated before using them for model evaluations, even when the parameters have a physical meaning. Even with the best model structure, parameter estimation will retain a residual uncertainty (Beck 1987), while will propagate forward into model predictions and the evaluation of management practices. In addition, many parameters in an environmental model are empirical quantities, which are entirely subject to the process of identification and calibration, directly or indirectly. The process of calibration will itself introduce uncertainties into parameter values, due to the limitation of monitoring data or inadequate background information. The possible temporal and spatial variability of parameters make it even harder or impossible to obtain their "true" values.

For instance, for a spatially distributed parameter, which is often the case for watershed modeling, the distributed parameter must be extracted by some form of averaging over the modeled spatial unit, for example, a small sub-basin or HRU. In addition, most parameters are assumed to be temporally constant in the model structure, while in the natural environmental systems, a large number of commonly used parameters are actually varying with time. The difference between the "true value" and our estimated values is one significant source of uncertainty in environmental modeling. Furthermore, even the most complicated environmental model contains quite a few empirical equations, such as Manning's Equation or Darcy's Law in hydrology, therefore, such that the parameter estimates associated with them cannot be transferred from one case study to another. Moreover, as we mentioned, most of the currently popular watershed models are to some extent over-parameterized, especially for those with a distributed structure where different parameter values are employed for each individual compartment due to the fact of spatial variability. Since in many cases parameter values cannot be obtained by field monitoring or lab experiment, this too brings more difficulties to achieving an adequate identification and might impair the reliability of the model evaluation.

(3) Predictive scenarios

In many cases, the ultimate target of environmental modeling is that of future behavior prediction. Scenarios are a wide variety of possible assumed conditions (for the future) that are affected by many uncertainties. Considerations of uncertainty in scenarios help link uncertainty about the future to decisions required today. In the process of future prediction, the external or internal factors which drive the system evolution need to be first predicted as inputs to the model application. These predictions are often generated according to the development plan for the area of interest. For example, for a watershed environmental quality prediction, population trends, economic development patterns, land-use trends, projected or being implemented pollution control plans, even climate change, are all required to be carefully examined.

This kind of uncertainty is also difficult to reduce. In this research, such scenario uncertainty is expressed by parameterization as well. For example, climate variation is parameterized as a dry, moderate, or wet hydrological year; the development scenario is parameterized according the regional plan of the given district; and the effectiveness of watershed pollution control actions are parameterized as a percentage that accounts for the success in attaining designed target performance.

(4) Data limitations

Monitoring data are the foundation for environmental systems analysis. The application of watershed and water-quality models involves substantial uncertainty as model parameters are sometimes estimated from inadequate data. The uncertainties come from measurement limitations or data scarcity, since normally sparse water quality observations are available, and errors or disturbances of measurements also bring uncertainties to the dataset. Furthermore, even when well-designed experiments are implemented, the measurements are still to some extent the results of averaging for the spatial or temporal variability of natural systems. We always face the situation of sparse data, even in U.S., where it is normally believed that the quantity and quality of watershed monitoring data are relative good. In actual projects, we often have to deal with observations that are inadequate, discontinuous, or inconsistent. For example, for phosphorus monitoring, multiple indices are adopted in real projects, including total phosphorus (TP), TP-filtered, total reactive phosphorus (TRP), orthophosphate, phosphate, soluble reactive phosphorus (SRP), and so on.

This problem exists in not only the process of data collection, but also in data preprocessing. Some hydraulic water quality indices are obtained by indirect measurements; for example, river discharge is estimated with the flow-stage relationship, and the concentration of total suspended solids is often generated based on the observation of turbidity with a transform equation. Such processing functions could bring more uncertainty into the data series. Another example could be that, for the spatial data of land cover type, which is the most important factor in the modeling of watershed nonpoint source pollution, the spatial distribution of land cover condition is obtained from a procedure of photographing or remote sensing, image processing, classification, onsite information gathering, image interpretation and map compilation, all of which bring more uncertainties. Similar conditions apply to soil data and topographic maps. In practice, most models use the dominating (above a threshold) soil type to represent the given basin, and ignore the influence of minor soil types.

Based on the discussions above, if we want to reduce the uncertainties in environmental modeling, we can consider several options such as model structure optimization and improvement, investigation to get more accurate parameter values, better scenario predictions, higher-quality monitoring. Among these the last one is likely to be the most promising.

3.2.3 Sensitivity analysis

Uncertainty and sensitivity analysis are applied as powerful tools for quality assurance in modeling and forecasting and their importance has been widely acknowledged in recent years. Sensitivity analysis (SA) is the study of how the variation in the output of a model can be apportioned, qualitatively or quantitatively, to different sources of variability in model inputs and parameters. Compared with uncertainty analysis, sensitivity analysis provides more information on the modeling system than the single analysis of outcome uncertainty. It helps modelers to appreciate better the inner workings of model structure. In brief, while uncertainty analysis refers to the determination of the uncertainty in model results that derives from uncertainty in model inputs, sensitivity analysis refers to the determination of the contributions of individual uncertain inputs to the uncertainty in model results (Helton et al. 2006b). These two approaches are often employed jointly.

In this dissertation, our approach to uncertainty and sensitivity analysis is as follows. For those parameters found to have high sensitivities, their variations will result in high impacts on the variation of model outputs. Then the uncertainty of the corresponding factors or processes will weaken the confidence in the simulation results. Sensitivity analysis also works to assist in the task of identifying the structure of the environmental system being investigated, by showing which components are dominant, or key processes, in hypothesis testing through model development (Osidele and Beck 2001).

In addition, where much uncertainty exists in the observation data, a so-called targeted monitoring can be conducted by specifically designing the measurement campaigns (Vandenberghe et al.

2007). Based on the results of sensitivity analysis, further monitoring efforts can be focused on the more significant factors for achieving a more effective reduction of the uncertainty and forecast error, through follow-on (refined) observation. This is important in practice for determining post-implementation monitoring priorities for a watershed, when used within the innovative scheme of adaptive water quality management under uncertainty (Harrison 2007; Shabman et al. 2007).

3.2.4 Approaches for UA/SA

Uncertainty is often described and measured as a probability distribution (Morgan and Henrion 1990), and analyzed with statistical approaches. Probability and statistics are natural elements of uncertainty analysis, because probability distributions can characterize the stochastic components of inputs to the phenomenon under study, while descriptive and inferential statistics provide information on the resulting outcome variables (Helton et al. 2006a; Piegorsch and Bailer 2005). They are also the principal tools in this dissertation.

From the foregoing survey, we see that for uncertainty and sensitivity analysis in environmental modeling a number of approaches, including both analytical and sampling-based methods, have been applied to investigate the propagation of uncertainty through a model system and to evaluate the effects of uncertainty on model outcomes. For relatively simple models and equations, a quantitative uncertainty analysis can be performed using analytical methods for statistical error propagation. These general analytical methods include differential analysis methods, first-order approximation, linear regression, Taylor expansion-based methods, Bayesian network models, variance decomposition (Sobol 1993).

The application of large complex and nonlinear models requires the adoption of more powerful approaches to account for uncertainties. With the rapid enhancement of computer technology, numerical or sampling-based approaches are increasingly becoming common tools for uncertainty analysis (Helton et al. 2006b). These sampling-based methods mainly include Monte Carlo simulation (MC), Latin Hypercube Sampling (LHS), Fourier Amplitude Sensitivity Test (FAST), Reliability Based Methods (FORM and SORM), Stochastic Response Surface Methods (RSM), Uniform Covering by Probabilistic Rejection (UCPR), Multiple Predictor Smoothing Methods (Storlie and Helton 2006), Markov Chain Monte Carlo (MCMC) (Gallagher and Doherty 2007), Generalized Likelihood Uncertainty Estimation (GLUE), and Regionalized Sensitivity Analysis (RSA).

Among these uncertainty and sensitivity analysis approaches, Monte Carlo simulation is considered the most applicable for complex environmental models (Hammonds et al. 1994; Helton et al. 2006a). In spite of the huge computational burden often required in practice, Monte Carlo simulation is still the most widely used form for environmental modeling research, because of its robust, distribution-free, easy-to-apply property. Monte Carlo simulation is a numerical method for generating simulated data using random numbers and assumed probability distributions to reflect the uncertainty in model inputs, parameters, and the model equations. It is rather suitable for the task of simulating the behavior of watershed systems with prominent stochastic processes, while the feasibility of other methods will inevitably be less, because of the nonlinearities, discontinuities, analytical intractability and complicated parameter interactions within such models.

Beginning in the 1990s, the U.S. EPA investigated methods for uncertainty analysis and issued guiding principles to encourage application of the Monte Carlo approach as a formal approach for uncertainty assessment in environmental modeling (EPA 1997). Since then, the Monte Carlo approach has been more widely adopted and many derivative approaches are developed for environmental systems analysis, such as RSA or GLUE. The basic algorithm of Monte Carlo simulation employs the algorithm of random sampling according to the predefined distribution of the uncertain factors and model inputs, and then in conjunction with the successive models runs, the propagation of uncertainty is expressed and their influence evaluated on a statistically significant distribution of model outputs. Therefore, the behavior of natural systems with uncertain processes is rather directly simulated.

However, even if there has been a consensus for years that uncertainty analysis is very important in environmental systems analysis, a large proportion of modeling studies still lack adequate exploration of uncertainty. There are some obstacles to the application of uncertainty analysis in environmental research, especially for the incorporation of uncertainty analysis into the decision process (Pappenberger and Beven 2006). Among these barriers, the most significant could be the absence of mature guidance on the relevant methodology and a universally applicable framework of practical uncertainty analysis. Although many approaches have been applied for uncertainty analysis in a number of case studies, there still remains a major challenge in redressing the lack of systematic uncertainty assessments to appropriately account for the uncertainties of both the modeling and decision-making phases. This will be a central concern in this dissertation.

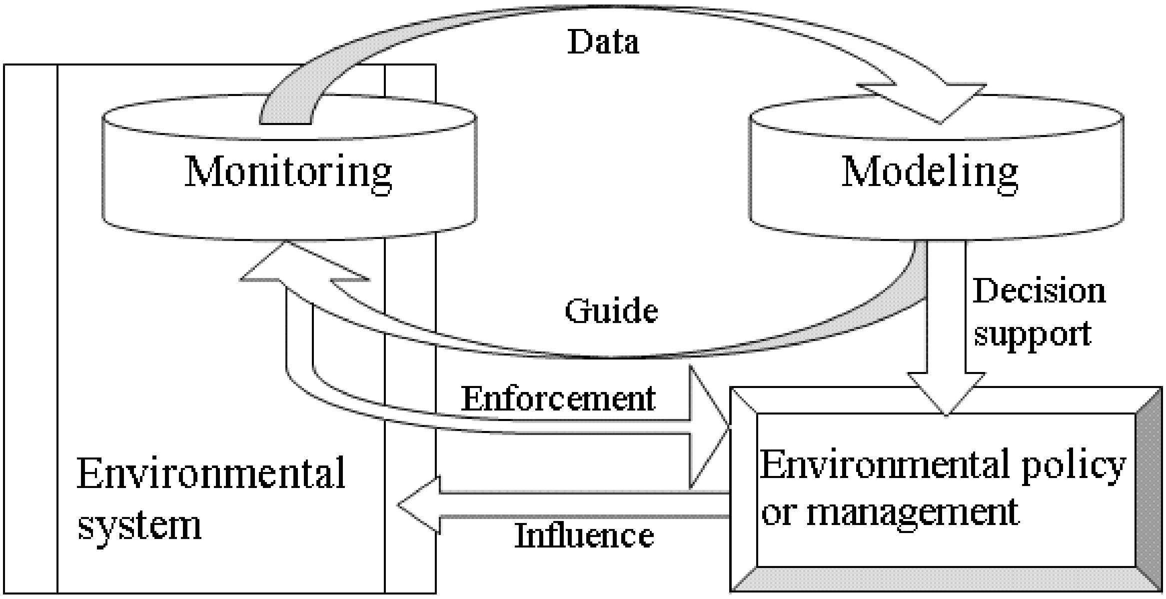


Figure 3-1: Components in environmental system analysis

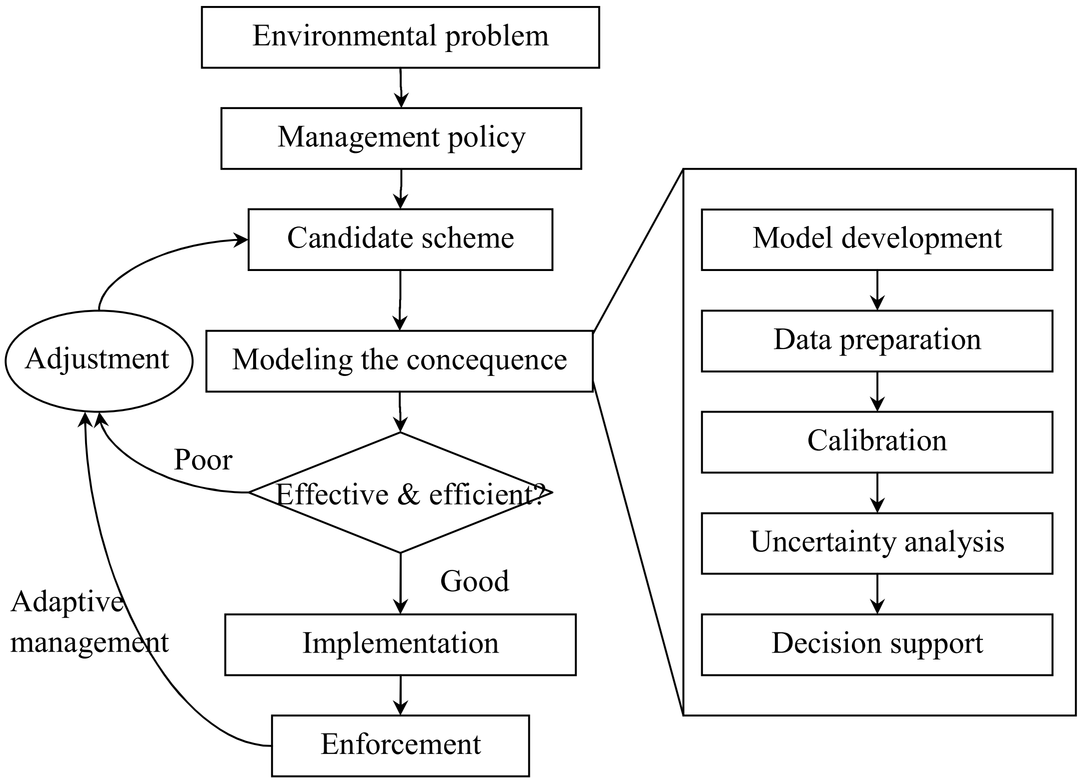


Figure 3-2: Modeling for environmental management

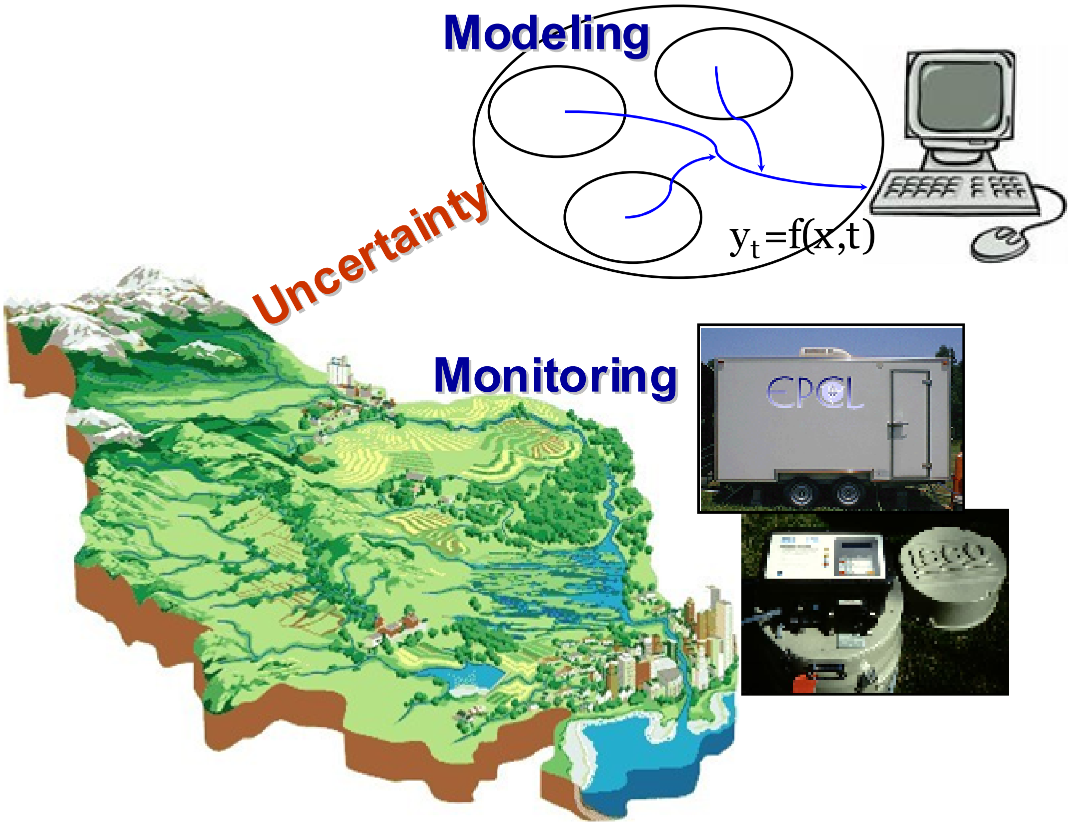


Figure 3-3: Uncertainties occur in model development

Chapter 4

PROCESSING THE UNCERTAINTY:

A COMPUTATIONAL METHODOLOGY

4.1 The approach of RSA

As we mentioned in previous chapters, a number of approaches are applicable for the task of uncertainty and sensitivity analysis associated with modeling research. Among them, the approach of Regionalized Sensitivity Analysis is a rather unique one (Saltelli et al. 2004). Essentially it is a Monte Carlo filtering algorithm used to study the significance of parameters and identify which is most or least sensitive, under a predefined condition of parameter variability and model structure. Through the reminder of this dissertation, the RSA approach is extensively employed.

Key RSA features are a random sampling process and a binary classification scheme. RSA first samples parametric values based upon pre-defined probabilistic distributions, which represent the prior parametric uncertainties, performs a number of model evaluations with these values, and then splits the model outputs into two subsets: those regarded as “acceptable” (i.e. result values fall within certain constraints), and those considered “unacceptable”. Accordingly, the values of the input parameters will be classified as two subsets, named “behavioral” and “nonbehavioral”, depending on whether they have produced acceptable or unacceptable model outputs. Subsequently the difference between the distributions of the “behavioral” and “nonbehavioral” parameters sets is evaluated to reveal the sensitivity of each parameter. Here the index of the

Kolmogorov-Smirnov (K-S) two-sample test statistic is often calculated for representing the difference between these two subsets, to show whether the distributions of the "behavioral" and "nonbehavioral" values of a parameter are significantly different. The higher the K-S index for any parameter, the higher its influence is on model response, with respect to discriminating whether the predefined behavioral condition is given or not. Because RSA employs the parameters as surrogates for the processes (the constituent hypotheses) described in the model's functional representations, a key system process is identified by the sensitivity of its respective parameter(s), through this RSA-KS method.

In the following paragraphs, since the approach of RSA is one of the emphases of this dissertation, we will introduce its definition, conceptual foundation, and discuss the numerical stability of this method when it is applied with the K-S test statistic. Fro this the limitations of the current RSA-KS algorithm will be revealed. All these efforts are aimed at developing the RSA methodology into a universal approach for uncertainty and sensitivity assessment in environmental modeling. This chapter primarily expresses our explorations of these theoretical issues, whereas the computational case study for illustrating its applications will be delivered in subsequent chapters.

4.2 History and previous relevant research

The Regionalized Sensitivity Analysis was developed in the late 1970s by Hornberger, Spear, and Young (Hornberger and Spear 1980; Hornberger and Spear 1981; Young 1978). Its first notable illustration was in a case study of cultural eutrophication in Peel Inlet, western Australia. Since then, it has been successfully applied in a number of environmental modeling studies. For example, it was used for quality assurance of a multi-media model for predictive screening tasks (Chen and

Beck 1999), for the identification of model structure and for investigating the behavior of lake aquatic ecosystem (Osidele and Beck 2001; Osidele and Beck 2004), for coping with the uncertainty in sediment transport and nutrient load analysis, and for examining the parametric uncertainty in water quality models (Osidele et al. 2006). Generally, it is regarded as a method particularly suitable for model identification and for assessing the quality of environmental models to assure the quality, or the trustworthiness, of a model's performance (Beck 1987; Beck 2002).

From its history, we see this approach was originally developed to provide research implications for a poorly understood estuarine ecological system, and to identify model structure in complex hydrological and environmental systems (Stigter and Beck 1994). One purpose of making good use the RSA approach is to incorporate into the model all relevant possible scientific hypotheses about what is causing a system to behave in the way observed, or closely tied to the qualitative subjective, field experience of scientists. Based on this the model could be deliberately composed to incorporate such features, addressing more questions of the important scientific hypotheses affecting the system behavior. Subsequently RSA has been increasingly used for investigating parametric uncertainties. RSA has been applied for estimating time-varying model parameters (Beck 2002). Another example could be that for the identification of a suitable model structure and the estimation of parameter values through calibration against observed data, a new approach called dynamic identifiably analysis (DYNIA) is derived from the RSA method for the identification and analysis of conceptual hydrological models (Wagener et al. 2003)

More significantly, by connecting three sampling-based computational approaches of RSA, TSDE (Tree-Structured Density Estimation) and UCPR (Uniform Covering by Probabilistic Rejection), a framework of Random-search Inverse Methodology for Model Evaluation (RIMME) (Osidele 2002) has been developed, as a novel methodology working in a backward pattern to identify the attributes of the model, and the corresponding real environmental system, that are critical to attaining a prescribed endpoint in the future (Beck et al. 2002; Osidele and Beck 2003). In contrast to the normally used forward pattern, from gathering the data to developing a model, and then to making predictions of future behavior, it is a reverse pattern of determining whether future conditions, as imagined by stakeholders or as specified by policymakers, are technically "reachable" given our current understanding of the environmental system. RIMME is considered a significant advance in shifting the enquiry to considerations of future behavior definitions (e.g. desired, to be regulated, or feared) including consideration of public perceptions of environmental behavior. Nowadays, since taking into account the perceptions of stakeholders is regarded as crucial to effective water quality management (Fath and Beck 2005), this backward methodology could play a substantially beneficial role for achieving scientific management. It can respond to the question of which elements of policy, or technology, and scientific hypotheses are critical or redundant in leading to the reachability of stakeholder-derived futures.

The major task of the RSA approach when it was originally invented was that of "hypothesis generation" in profoundly data-sparse situations. Most of subsequent successful studies have been similarly directed, and RSA has displayed good performance in these cases. However, as a universal method, it should not be confined to the data-sparse cases. It is considered to be qualified as well under data-rich conditions, for the purpose of exploring highly dynamic system behavior in association with high-frequency data and model applications.

4.3 A different form of sensitivity

The term RSA shows us that it is, after all, an approach to sensitivity analysis. At present, the topic of sensitivity analysis is usually expressed in two distinct forms: local sensitivity analysis (LSA) and global sensitivity analysis (GSA). LSA studies the model sensitivity in the vicinity of a certain parameter vector, i.e. the impact on the model output subject to small changes in one or multiple parameters. Meanwhile, GSA evaluates the parametric sensitivity across entire ranges of parameter values. In recent decades, these two forms have been extensively applied in modeling. However, rather different to these two SA forms, the so-called "regionalized" sensitivity analysis also plays a notable role in environmental systems analysis.

According to the above definition of RSA, we believe it is especially suitable for some specific tasks, such as management-oriented uncertainty evaluation or model calibration under uncertainty. The idea of defining an "acceptable" range for model outputs is particularly compatible for these kinds of problems, where system behavior is assessed according to some constraints. For example, for water quality problems, we can define the desired target behavior (of the model outputs) as that actual water quality compatible with the regulatory standard. This is practically useful to investigating the impacts of relevant factors on the attainment of a water quality standard, that is, how the factors' variations will affect the simulated outputs of water quality by forcing model outcomes to meet or violate the required standard, e.g., pollutant concentration limit. Another rather suitable platform is in the process of model identification or parameter calibration. We know an important task of sensitivity analysis is to show whether, and how significantly, the parametric variation will affect the model output with respect to whether the observed data are matched or not. By means of defining target behavior in terms of the model outputs being reasonably close to the measurements, the sensitivity of each parameter affecting the reconciliation of simulation and observation can be evaluated.

In such cases, the acceptable model output is determined by the predefined system behavior and, accordingly, the behavioral values of parameters are distributed in a certain region of the parametric space. The term “regionalized sensitivity” can be considered as being derived from this process. It is regarded as a new form of sensitivity, conditioned by system behavior and regionalized within the behavioral/nonbehavioral parametric space. In contrast, GSA is intended to reveal how the factors’ variation affects the model output across the entire range of feasible parameter values, thus being called “global” or “unconditional” sensitivity. Figure 4-1 illustrates the distinct features of LSA, GSA and RSA. Figure 4-2 is a further schematic illustration of the workings of RSA.

The conceptual explanation of the RSA method described here might differ somewhat from its original definition, when it was first introduced thirty years ago. Instead of considering it as a simple algorithm for a special task of environmental modeling, we would prefer to define regionalized sensitivity as a more general concept, complementing local and global sensitivities. We suggest that for those conditions mentioned in the preceding paragraph, the regionalized sensitivity and its analysis method are more suitable, and therefore attractive, both theoretically and practically, than the global form.

The entire computational algorithm of the RSA comprises the process of random sampling, binary classification, and sensitivity index calculation. We know that the local sensitivity index is usually expressed by the first-order response slope (or first-order difference): $S=(f(x+\Delta x)-f(x))/\Delta x$. One-factor-At-a-Time sensitivity analysis is an algorithm based on this concept that is used widely to evaluate the variability of model results as a function of each individual parameter. Global sensitivity is a more complex form and is normally expressed as different types of correlation coefficients, correlation ratios, or Sobol's indices (Kurowicka and Cooke 2006). As mentioned above, the regionalized sensitivity is often measured with the index of K-S statistics, especially through the RSA-KS algorithm.

4.4 Comparison with the GLUE method

Generalized Likelihood Uncertainty Estimation (GLUE) is another algorithm even more widely used in the area of hydrological modeling and uncertainty analyses (Beven 1989; Beven and Binley 1992; Zheng and Keller 2007). In GLUE, modeling errors associated with each acceptable model parameterization (and structure) are treated implicitly, under the assumption that error series associated with a particular model will be similar in prediction to those found in evaluation or calibration. Each model run can be given a likelihood weight to express relative belief in that particular model, based on the evaluation of the model performance for a calibration data set. Each acceptable model run will be considered in prediction according to its weight (or likelihood).

In short, we may say that RSA and GLUE have some similarities, but their difference are also significant. In RSA, each parameter vector in the behavior-giving set is assumed to have an equal likelihood of generating the acceptable behavior; RSA is giving each behavioral parameter vector the same probability of $1/m$ (m is the number of behavioral parameter vectors). In contrast, the GLUE method evaluates the likelihood of a model run generating the desired simulations results (likelihood is determined by the difference between the simulation and observation, where a higher likelihood is assigned when the simulation is closer to the observations), It assigns each parameter set an index or likelihood weight, and the posterior probability is derived from both acceptable parameters and their likelihood.

The advantage of GLUE over RSA is that it utilizes all the information of model realizations, by taking into account each realization's fitness as a weight, while RSA neglects the differences between simulation results within the behavioral and nonbehavior sets. RSA might be considered as a specific form of GLUE, wherein a uniform likelihood measure of $1/m$ is adopted for each behavioral parameter vector and zero for all nonbehavioral ones. GLUE is closer to a GSA computational approach. Compared with GLUE, RSA is apparently easier to apply, more suitable to data-sparse conditions, as well as to the decision-oriented modeling studies because of the involvement of constraints such as an environmental standard, as mentioned in the proceeding section. We believe, therefore, that RSA is more suitable to be applied in this study.

4.5 Working procedure

Application of the RSA-KS algorithm often includes several major steps, which are listed below and schematically displayed in Figure 4-3. The case study illustrated in subsequent chapters generally follows these steps. Three important elements in this approach are further explained and discussed below.

(1) Define the constraints for target system behavior, based on environmental foresight, stakeholders concerns, water quality standards, or field observations (for calibration);

(2) Specify the prior distributions of the model parameters, accounting for epistemic uncertainty and possible variability of external or internal factors (aleatory uncertainty);

(3) Sample randomly (with a pure or stratified sampling algorithm) according to the prior parametric distribution;

(4) Substitute the sampled parameter vectors into the model, run the model for a number of replications, and generate model output trajectories for evaluation;

(5) Classify the outputs between an "acceptable" set (*m* elements) and an "unacceptable" set (*n* elements), and consequently classify the parameter vectors as "behavioral" and "nonbehavioral" sets;

(6) Compare the difference between "behavioral" and "nonbehavioral" parametric distributions by calculating the Kolmogorov-Smirnov two-sample test statistic (*d*), or its standardized form (*Z*), for each parameter, as the sensitivity index;

(7) Categorize each parameter into critical and redundant groups according to their significance or sensitivitity;

(8) Draw conclusions about the importance of each factor in the corresponding real system based on their relative sensitivities expressed by the magnitude and rank of *d* or *Z*, and identify the critical factors or important component processes.

4.6 Important elements

4.6.1 Sampling strategy

Sampling is the first step and "driver" the computational algorithm in the RSA approach. It is usually performed through two random sampling strategies: simple (or pure) random sampling and stratified sampling. Monte Carlo Simulation is a typical scheme of pure random sampling, and

Latin Hypercube Sampling (LHS) is one of the most popular algorithms of stratified sampling. These two schemes will be essentially examined in this section.

Pure random sampling means that every possible sample has an equal chance of being selected from the population. It is a good approach for simulating the uncertainty represented by some probability distributions, except for the disadvantage of the huge time and computational resources often required for large models. With sufficient sampling points, the sample will make an exact description of the uncertainty of interest, and thus increase the stability of the subsequent simulation process. This is the primary reason for which we usually need to generate a large number of sampling points when using a numerical approach such as Monte Carlo Simulation. Because it can be very time-consuming, some special sampling techniques have been developed and employed for improving computational efficiency. Their goal is that with a lower number of sampling points, the sets of random vectors become a better representation of the variability or uncertainty (regarding mean and variance, for example).

Among the strategies for improving the computational efficiency. Among them, Latin Hypercube Sampling is widelyused, stratified sampling algorithm for uncertainty analyses (Helton and Davis 2003; Iman et al. 1981). In this method, the range of probable values for each uncertain input parameter is divided into ordered segments of equal probability. Thus, the entire parameter space, with one or multiple dimensions, is partitioned into divisions that have equal probability, and they are sampled such that each parameter is sampled once (or equal times) from each of its possible segments. The advantage of this approach is that the random samples are collected from all the ranges (each division is sampled) of possible values, thus generating a “more complete” probability distribution of the parameter values. Compared with simple random sampling, the algorithm of LHS can approximate more effectively the underlying probabilistic distribution with fewer sampling points and subsequent model runs.

The RSA approach can incorporate any sampling scheme to generate parameter samples from the prior parametric distribution for model evaluation. If the parametric sample set has a size of N vectors, after running the model for N replications with these parameter values, the generated N model results, by which a probabilistic distribution of model outputs can be derived, reflect the variation of system behavior given the uncertainties of these factors.

In fact, Latin Hypercube Sampling instead of pure random sampling has been employed in some significant previous studies with RSA (Osidele et al. 2003; Osidele et al. 2006). It is expected that LHS will generate collections of parameter values that are closer to the underlying true distribution and consequently lead to more stable results for the RSA-KS algorithm. However, this advantage is to some extent impaired when samples are generated from a joint distribution of parameters, which will be necessary for two or more parameters. In this study, we have conducted trial computations with both pure and stratified sampling (LHS) for driving the RSA-KS computation, in which our computational results have shown that pure sampling and LHS do not differ significantly in calculating results of the sensitivity index with the same sampling size. Thus they have approximately equivalent computational efficiency.

4.6.2 Behavior definitions and binary classification

Generally, two types of behavioral definition are employed in the RSA. For model calibration, we usually assign the behavior definition such that model outputs fall within some bounds reasonably close to the observed data. Normally an objective function is defined to assess the discrepancy between the model output and observed data. A typical form of objective function is their distance $D(Y_{sim}, Y_{obs})$, or some type of goodness-of-fit index of a model application $C(Y_{sim}, Y_{obs})$. The simulation target, or acceptable system behavior, will be that the distance is not great (less than a threshold D_0), $D(Y_{sim}, Y_{obs})<D_0$, or the calculated model fitting coefficient is larger than a threshold, $C(Y_{sim}, Y_{obs})> C_0$. For other applications of environmental assessment or prediction, such as that of the RIMME framework, the acceptable system behavior is often defined as the model outputs are compatible with the environmental standard (such as an effluent or concentration limit), or they meet the requirements of stakeholders. According to these behavior definitions, each model evaluation associated with a parameter vector is then classified as exhibiting either behavior B or nonbehavior B^C, based on whether the model outputs meet these predefined constraints.

4.6.3 Sensitivity index

For revealing how much the variability in component entities will affect the behavior of the simulated system, the K-S statistic is calculated after the random sampling and binary classification procedure. It shows us the relative impact (thus importance) of the uncertainties associated with each parameter in the model and allows us to distinguish those critical factors from the redundant ones.

In statistics, the Kolmogorov-Smirnov test (often abbreviated as K-S test) is a widely-used method to determine whether two underlying one-dimensional probability distributions differ, or whether an underlying probability distribution differs from a hypothesized distribution, based on finite samples (Lefebvre 2006). In order to test for general differences between two distributions, it compares their sample CDFs (Cumulative Distribution Functions), using the maximum vertical distance between them as the test index. As a distribution-free approach, the two-sample K-S test is one of the most important and effective nonparametric methods for comparing two datasets, as it is sensitive to differences in both locations and shapes of the empirical cumulative distribution functions of the samples. In practice, the K-S statistic is both easy-to-manipulate and universal for testing general differences between any two distributions.

In this RSA-KS algorithm, we use the K-S test to explore whether, for a particular uncertain parameter or variable factor, the empirical probability distribution of parameter values within the behavioral set is significantly different from that in the nonbehavioral set. Here the hypothesis in K-S two-sample test is defined as:

H_0: $f_m(x_i|B) = f_n(x_i|B^C)$. The empirical probability distribution of the i^{th} parameter (X_i) in the behavioral set is NOT different from that in nonbehavioral set. This is the null hypothesis.
H_a: $f_m(x_i|B) \neq f_n(x_i|B^C)$. They are different. This is the alternative hypothesis.

Here the K-S statistic (d) is employed as the index to indicate the regionalized sensitivity of the parameters. It is calculated as

$$d(X_i) = Sup_y \left\| F(x_i|B) - F(x_i|B^C) \right\| \qquad (4\text{-}1)$$

where X_i (i=1,2,…,k) is the uncertainty-bearing parameter of interest; $F(x_i)$ is the prior distribution function being be sampled, defined according to the assumed parametric uncertainty or variation; m denotes the size of acceptable model realizations and n is the size of the nonbehavioral parameter set; the notation Sup_y is defined as the largest vertical separation between behavioral and nonbehavioral distribution functions (shown in Figure 4-4). $F(x_i|B)$ and $F(x_i|B^C)$ are the marginal cumulative distribution functions of the i^{th} parameter for m behavioral and n nonbehavioral values. From the parameter values in both sample sets, $F(x_i|B)$ and $F(x_i|B^C)$ are calculated with:

$$F(x_i|B) = \Pr(X_i \le x_i|B) = \frac{\sum_{p=1}^{m} T_{x_i}(X_{i,p})}{m} \qquad (4\text{-}2)$$

$$F(x_i|B^C) = \Pr(X_i \le x_i|B^C) = \frac{\sum_{q=1}^{n} T_{x_i}(X_{i,q})}{n} \qquad (4\text{-}3)$$

where $X_{i,p} \in B$ ($p=1,2,\ldots,m$) are the behavioral values for the i^{th} parameter; and $X_{i,q} \in B^C$ ($q=1,2,\ldots,n$) are the nonbehavioral values. T is a mathematical operator which is defined as

$$T_a(y) = \begin{cases} 1 & if(y \le a) \\ 2 & if(y > a) \end{cases} \qquad (4\text{-}4)$$

The calculation of the K-S statistic d is shown in Figure 4-4. It is the maximum difference between two cumulative distribution functions: the green curve, for $F(x_i|B)$ and red curve, for $F(x_i|B^C)$. The blue line is the cumulative distribution function curve of the entire parametric sample, which corresponds to a uniform distribution, shown as a straight line in this case.

4.6.4 Standardized K-S statistic

As a statistical hypothesis test, in order to obtain support for the alternative hypothesis, we need to calculate how likely (how often) we would obtain results as extreme as the calculated values in a test. For this purpose, we need to investigate the probabilistic distribution of *d* under the null hypothesis (when the null hypothesis is the reality). We have conducted a computational experiment to explore the statistical properties of the *d* value, from which it can be shown that when in reality these is no difference between two underlying probabilistic distributions, which means two sampling sets are taken randomly from identical distributions, the calculated value of *d* is a function of the sample size.

Figure 4-5 demonstrates the expectation and standard deviation of the K-S statistic *d* when two random samples are generated from the SAME underlying distributions, when the null hypothesis is actually true. Specifically, we sampled two random dataset separately (each with 500 points), but under same certain distribution functions, e.g. Uniform(*a*, *b*), by which the variable is uniformly distributed on the range between *a* and *b*, and then we calculate the *d* value for each parameter. The procedure is repeated without change of conditions, where we find the *d* value is varying for each replicated computation. Thus we repeat it a 1000 times (sampling two 500-point datasets on Uniform(*a*, *b*) and calculate *d*), so that these 1000 *d* values represent an empirical probability distribution, the expectation and standard deviation of which are plotted as one solid black circle and vertical bar in Figure 4-5. Next, we substitute the sampling size (N=1000) with different numbers such as 100, 200, …, 5000, from which the computational results clearly show that the expectation and standard deviation of the K-S statistic *d* varies accordingly.

Figure 4-5 has illustrated that with larger sample size, the expectation and variance of K-S statistic both become lower. Recall, however, that the purpose of the application of the RSA-KS algorithm is to highlight the characteristics of the given model and associated uncertainty issues. If, for a given combination of modeling and uncertainty consideration, the result of KS statistic (*d*) is varying with the sampling process, as shown in Figure 4-5, then we would say it is very necessary to introduce and employ some other, more "standardized" index.

This computational experiment has shown a distinct relation between the statistical properties of the *d* value and the sampling size (*N*): the expectation of *d* is dependent on *N* with an extremely high value of regression coefficient of 0.9997. This strongly implies that this relation can be perfectly expressed with some type of power-law equations, such that a mathematical change of form might generate a standardized index which is sampling-independent. When we check the expectation (*E*) and standard deviation (σ) of the *d* value, based on the numerical computation results, as shown in Figure 4-5, we have found that the calculated *d* value is exactly dependent on the number of behavioral and nonbehavioral simulations, *m* and *n*, with the following relation:

$$E(d) = C_{ks} \cdot P_{mn} \qquad (4\text{-}5)$$

$$\sigma(d) = D_{ks} \cdot P_{mn} \qquad (4\text{-}6)$$

$$P_{mn} = \sqrt{\frac{m+n}{m \cdot n}} \qquad (4\text{-}7)$$

The Equations 4-5 and 4-6 mean that the expectation and variance of *d* are in direct proportion to the operator of P_{mn}, with a invariant ratio of C_{ks}, and D_{ks}. A suggestion could therefore be that if the form of d/P_{mn} is taken to define an index, the new index would be independent of m and n. Thus the standardized K-S statistic Z is introduced, defined as

$$Z = d \cdot \sqrt{\frac{m \cdot n}{m + n}} \qquad (4\text{-}8)$$

Based on the above statements, we can easily obtain

$$E(Z) = C_{ks} \qquad (4\text{-}9)$$

$$\sigma(Z) \cong D_{ks} \qquad (4\text{-}10)$$

The computational experiment has shown that Z has a fixed distribution, with an expectation of 0.85 (approximation) and standard deviation of 0.25, when the reality is that the distributions underlying (to-be-tested) two samples are not different. Its cumulative probability distribution is displayed in Figure 4-6. Therefore, in the two-sample K-S test, the standardized K-S statistic Z is a sample-independent index. Figure 4-6 also displays the critical region that represents the extreme evidence against the null hypothesis. The probability of the test statistic falling in the critical region when the null hypothesis is true is called the "alpha" value of the test. It is the probability of the extreme event happening so that we can reject the null hypothesis, and represents the significance level of this test. We need to choose a significance level for each test.

From Figure 4-6, we can derive the critical value for the K-S statistic at different significance levels, such as 0.1, 0.05 and 0.01. They are listed in Table 4-1. After the test statistic Z is calculated by the RSA-KS algorithm, we refer to Table 4-1 to determine whether it is inside the critical region. If the value of Z is larger than the critical value (e.g., $Z>1.52$, given $\alpha=0.01$), it means an event of probability less than alpha has occurred, and the hypothesis H_0 is incorrect. Therefore, we will reject the null hypothesis and conclude that these two sample sets are statistically different and that the corresponding uncertain factor is important. If the test statistic is outside the critical region (less than the threshold), the conclusion is that there is not enough evidence to reject the null hypothesis. We cannot say these two distributions are significantly different, and the corresponding uncertainty factor is judged to be less important or redundant.

In addition, the results generated by this numerical experiment also demonstrate important aspects of the research into the stability of the current RSA-KS algorithm. In some significant case studies, when it is applied to calculate the sensitivity indices of d and Z for evaluating the importance of each parameter under the condition of predefined input uncertainty and simulation targets, we often notice that different replications of the RSA computation can produce different results, even for the same prior uncertainty prescription (or parametric variation) and behavioral definition (Osidele et al. 2006). This point might impair the reliability of any subsequent conclusions drawn from the computational results of this approach, because of the lack of the repeatability.

The main reason for this phenomenon is that the RSA-KS algorithm is driven by the process of random sampling. When samples are taken from the predefined probability distributions, which reflect the uncertainty or variability of each parameter, these sample sets for the parameter values are not the exact analytical depiction of the underlying real distribution, but only a numerical approximation of it. It is similar to the condition of using the attribute of a subset to represent the whole ensemble, which will inevitably lead to a somewhat biased representation. Here we have explored and shown by Figures 4-5 and 4-6 how much confidence can be placed in our conclusions from sensitivity and uncertainty analyses.

Table 4-1: Critical values for the standard K-S statistic *Z*

Critical Value	Significance level (α)
1.95	0.05%
1.6276	0.5%
1.5174	1%
1.3581	2.5%
1.2239	5%
1.0730	10%

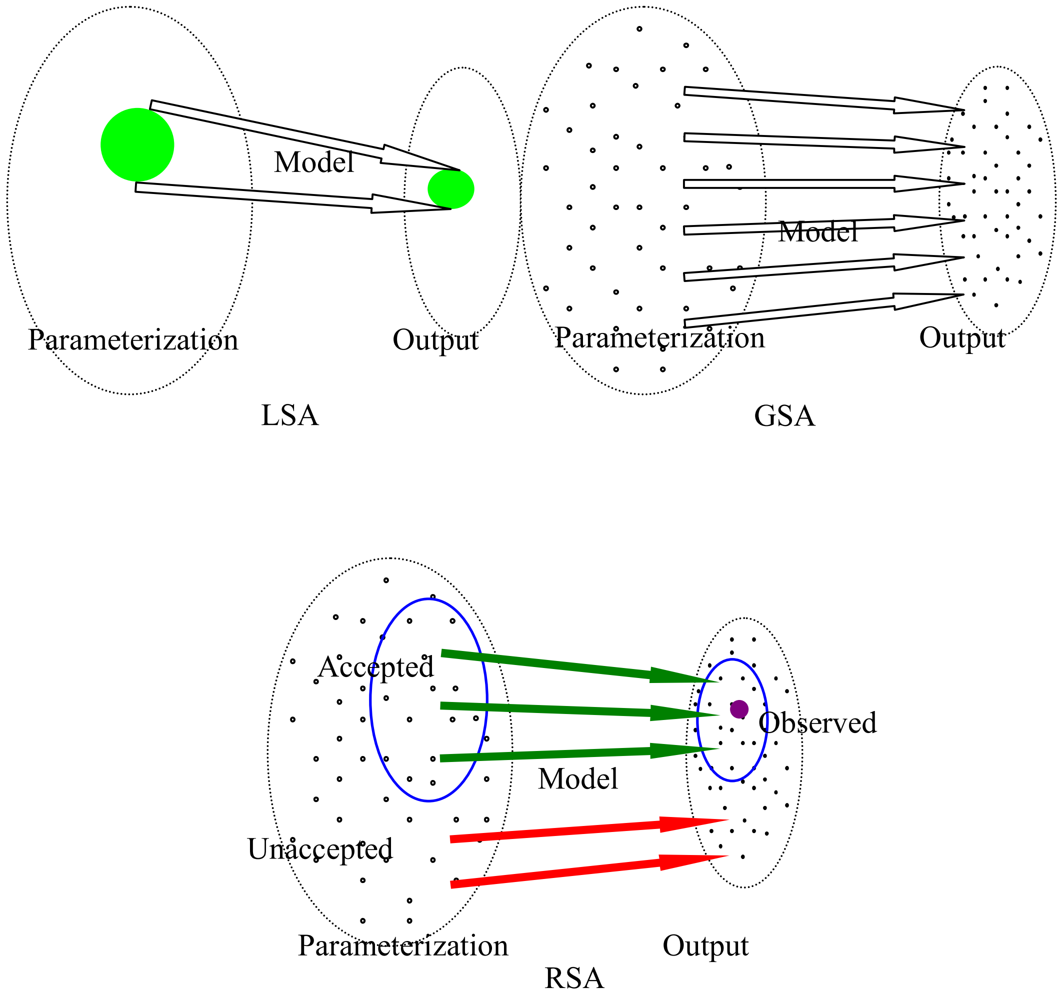


Figure 4-1: Three forms of sensitivity analysis

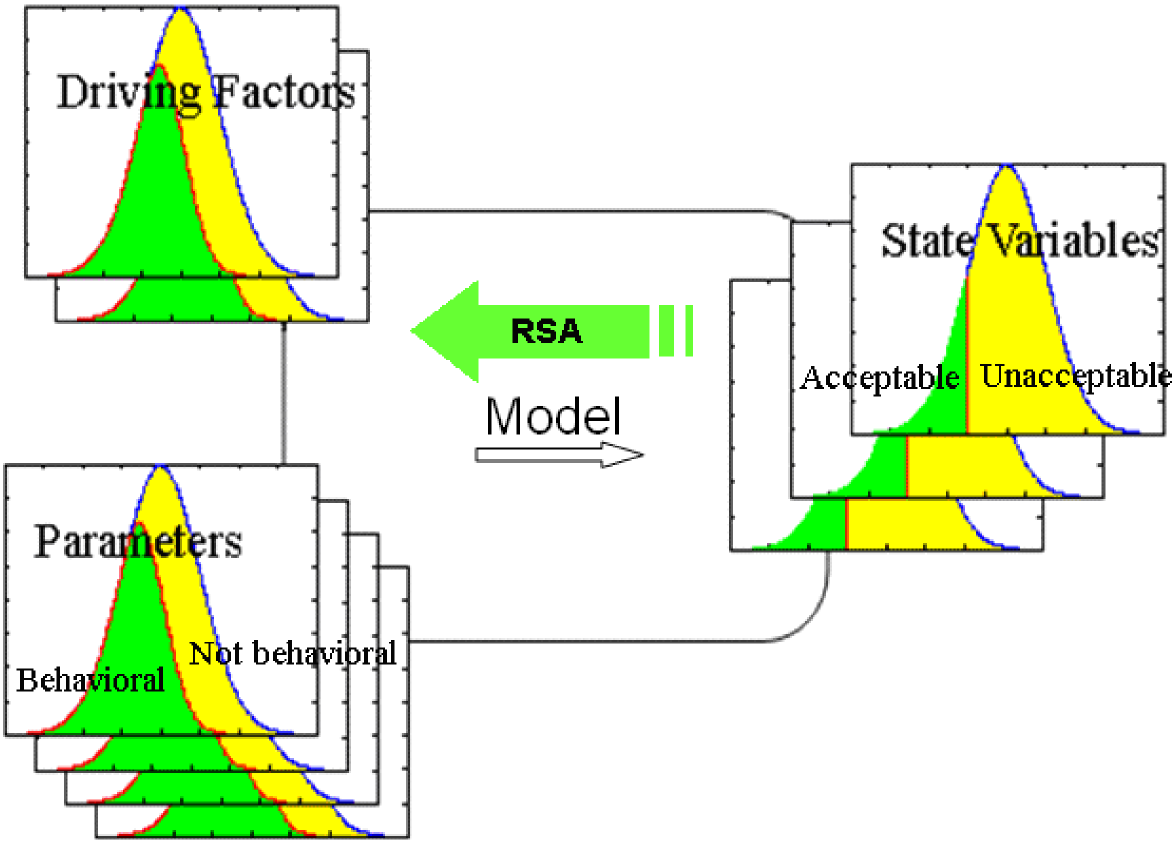


Figure 4-2: Uncertainty propagation and Sensitivity Analysis

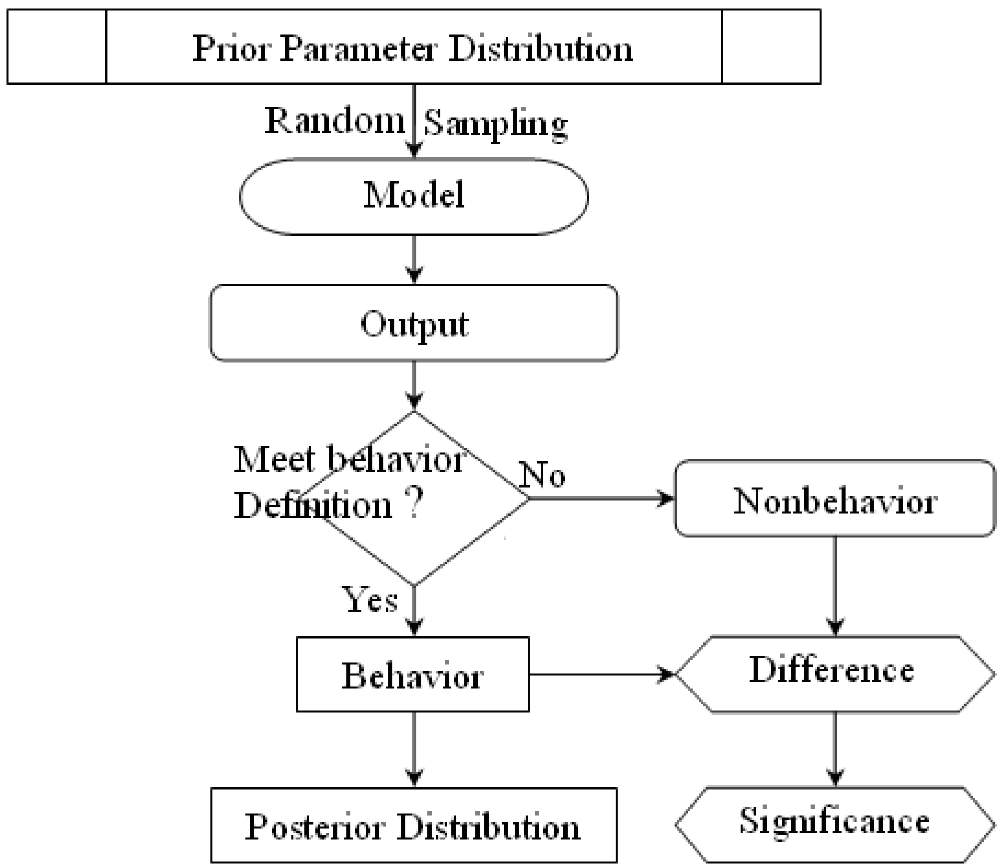


Figure 4-3: Procedures of RSA implementation

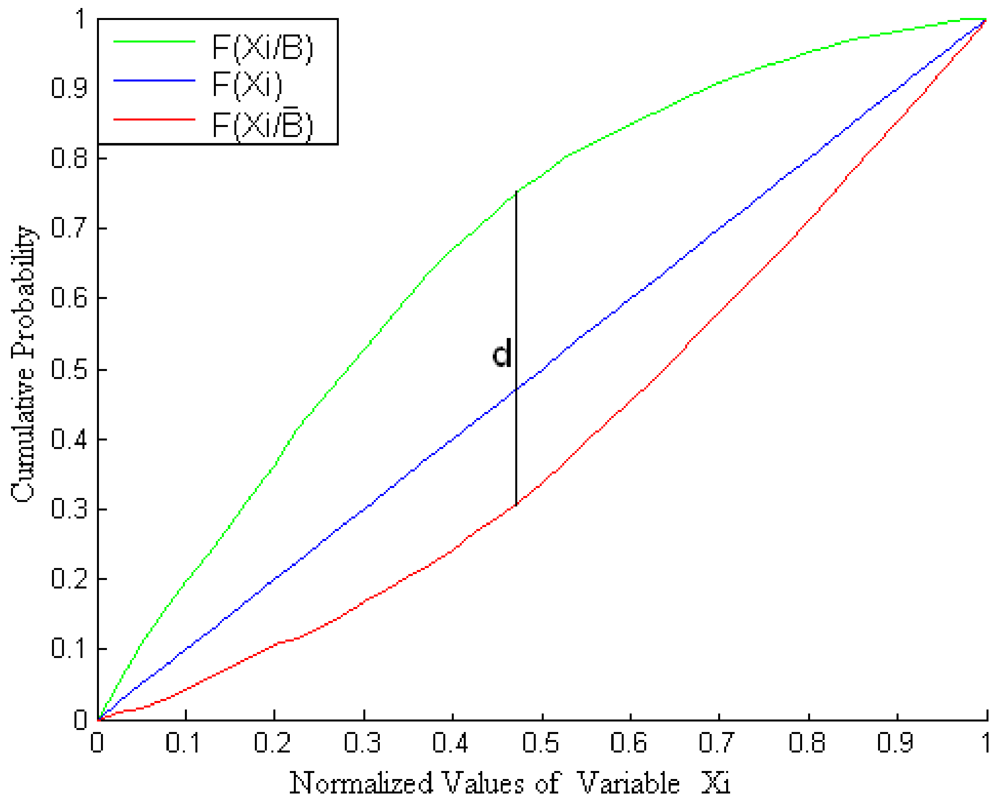


Figure 4-4: Graphical representation of the K-S statistic (*d*)

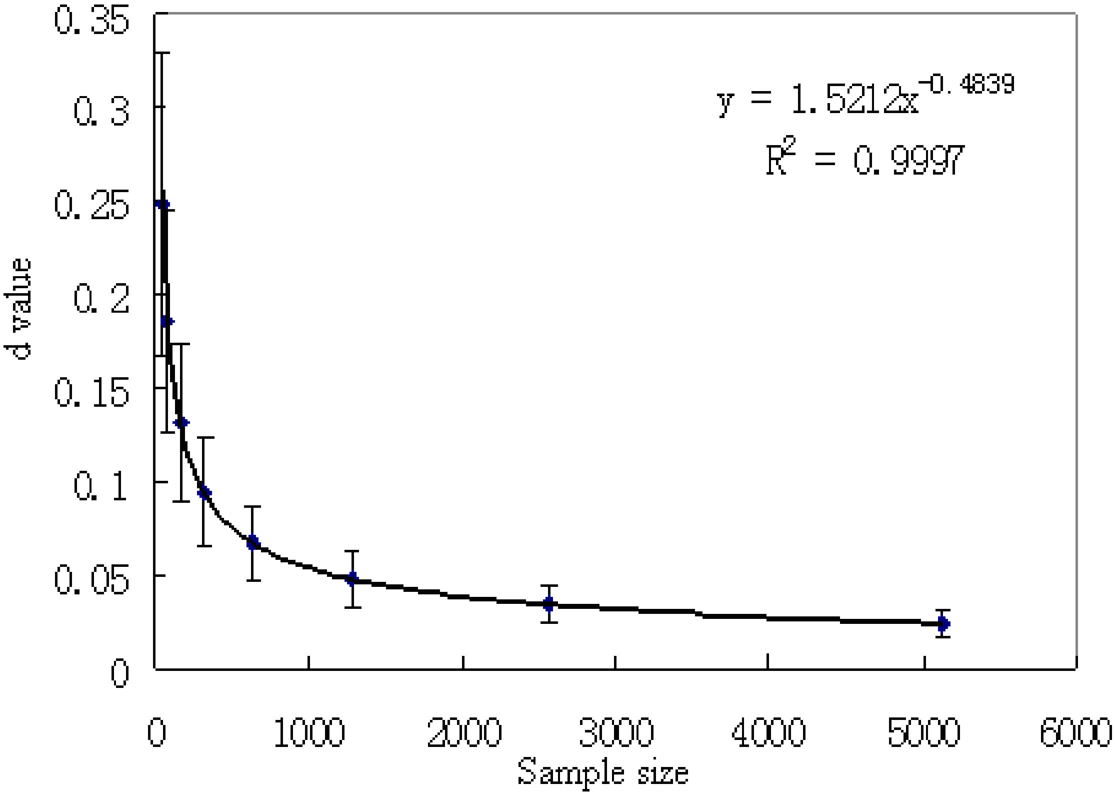


Figure 4-5: Expectation and Standard Deviation of *d*

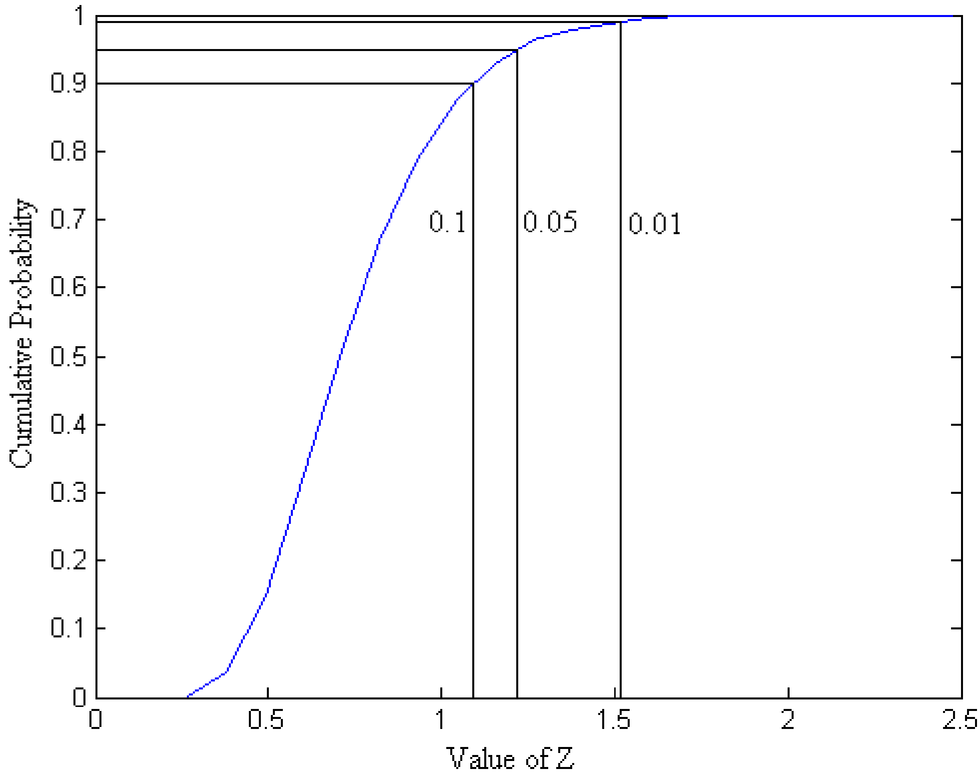


Figure 4-6: CDF of standard K-S statistic Z

Chapter 5

ASSEMBLING A WATERSHED SIMULATION SYSTEM AND ITS APPLICATION TO THE CHATTAHOOCHEE WATERSHED

5.1 Watershed systems analysis

5.1.1 An overview

Water resource and water quality research has been addressed from the perspective of the watershed for many years. Such research must be based on a comprehensive and accurate understanding of the given system, for which purpose we will first conduct an analysis on the influential external and internal factors, the incorporated processes, and the main features of the watershed system. Based on these, we can then propose an appropriate scheme for further scientific or management study.

There has been a consensus that the watershed system is an extremely complex system and description and prediction of its behavior are very difficult. A number of important factors interact with each other in the processes of the watershed hydrologic cycle, including precipitation, evapotranspiration (both evaporation and transpiration), surface runoff, infiltration, interflow, groundwater movement, and channel routing (Ward and Trimble 2003). Pollutant transport is associated with each of these processes and accompanied by multiple transformations, such as physical, chemical or biological immobilization and mobilization. Figure 5-1 illustrates the general hydrological and pollutant-associated processes in the watershed system.

Many factors influence watershed hydraulic and pollution behavior, primarily the terrain or landform, land use type, geologic and soil conditions, and so on (Carlsen et al. 2004), Human activity is also a significant factor, which affects the watershed environmental system through the changes of land surface conditions, municipal sewage discharges, and restorative and remediation actions. .

The complexity of the watershed system is mainly derived from three features: multiple and interacting component processes, highly dynamic mechanisms, and nonlinear relationships between factors and state variables. The hydraulic process of precipitation-runoff and water discharge is the basic process of watershed behavior. In this process, the runoff rate is determined by a nonlinear function of meteorological and watershed characteristics. The consequent process of stream routing inherits this feature too, always shown by both the time lag and shape change when we examine the hydrograph. As far as sediment is concerned, the processes of soil erosion, transport, deposition and resuspension reflect the complexity as well. For nutrients, the nonlinear pattern is more significant. In watershed modeling, nutrient transformation between different forms, the adsorption and desorption processes, and biologically mediated processes are often described by dynamic equations or even more complicated biological kinetics equations containing several feedback loops. Because of the high complexity of watershed processes, they need to be evaluated by powerful techniques. As a result, very large, comprehensive, and high-order watershed modeling approaches are developed and employed for exploring and describing the hydrologic and pollutant behavior of a watershed.

5.1.2 Pollution sources

With respect to the issue of water quality in a watershed, the sources of pollution are often of two major types, point sources and nonpoint sources, as also demonstrated in Figure 5-1. Point sources are mostly produced by anthropogenic activities, primarily including the municipal sewage system, wastewater treatment plants and industrial dischargers. Compared with nonpoint sources, which are primarily induced by the transient event of precipitation, point sources are more characterized by periodical cycles of both discharge rate and pollutant concentration, with a daily or weekly pattern, consistent with the rhythm of human society. At the same time, this will inevitably result in a disturbance of the temporal frequency spectrum and therefore the ecological metabolism of the natural aquatic system. Some of the power in the lower-frequency components of the watershed's hydrological and nutrient regime (with periods of millennia, centuries, decades, years, and seasons) is transferred to the higher-frequency components, fluctuating over weeks, days, and hours (Beck 2005b; Beck et al. 2008b). In addition, a major portion of the point sources are located within urban and surrounding areas. Their effect on the water body could be considered as reflecting the environmental impacts of cities. In the urban environment, environmental concerns focus on high-volume wastewater discharges and concentrated runoff from extensive impervious surfaces. Technically, estimations or predictions of point sources are often based on the population, season, water use type, water supply and discharge data acquired by monitoring, and the developing trends.

Nonpoint source pollution, in contrast to point sources, comes from sources spatially distributed throughout the entire watershed area. Nonpoint source pollution is induced by the process of precipitation-runoff, when rainfall or snowmelt water move over and through the ground. As the runoff moves, it picks up and carries away natural and human-made pollutants, finally deposits them into lakes, rivers, wetlands, coastal waters, and even underground sources of drinking water (EPA 1994). As a result, the discharge of nonpoint source pollution is primarily dependent on two aspects: meteorological and terrestrial conditions. In particular, land use and land cover exert a most significant influence, from the view of both local and global, short-term and long-term (Billen et al. 2007; Frick and Buell 1999; McCutcheon et al. 1993)

Compared to point sources, nonpoint-source discharges occur universally in conjunction with the precipitation-runoff process, such that they are hard to be directly monitored and accurately estimated. As a result, the study of nonpoint sources is highly dependent on the tool of watershed models. At the same time, the spatially distributed property of nonpoint sources also brings much difficulty for effective management and control. In fact, for the past several decades, as point-source pollution from municipal and industrial dischargers have become tightly controlled and substantially reduced by the wholesale implementation of wastewater treatment and strict regulations, the problem of nonpoint sources, still unregulated in most areas, is becoming increasingly significant. Generally in a watershed system, during wet periods, the water discharge rate and pollutant load is more likely to be dominated by nonpoint sources, while during the base flow periods water quality is mainly determined by point sources.

5.1.3 Phosphorus behavior

Phosphorus is an essential nutrient for plant growth. However, too much nutrient can have disastrous effects. The concentration of phosphorus in fresh water is usually low, but given excessive phosphorus release from watershed discharges into water bodies it can become a threat to water quality degradation and ecological impairment. Phosphorus behaves as the limiting nutrient for eutrophication in the U.S. Southeast, as well as many regions around the world, and is considered an important factor in the current degradation of surface water. Phosphorus problems often occur in lakes and reservoirs, but originally result from inputs from the upstream watershed. Application of fertilizer or manure in agricultural lands is the main source for high phosphorus loads. Paying close attention to the amounts and forms of fertilizer application makes therefore a difference in determining how much nutrients will be utilized by plants rather than lost to water bodies (Carlsen et al. 2004).

The main processes affecting phosphorus in a watershed include its accumulation in the soils surface, wash off, particle adsorption, desorption, deposition and entrainment with sediment, bio-uptake and bio-release. In soils, most phosphorus clings tightly to soil particles. Its dissolved phase is usually found in the form of phosphate (PO_4^{-3}), of which orthophosphate is the most stable form and the primary form used by plants. Hydraulic processes such as runoff and stream flow transport most of the total phosphorus. Significant phosphorus loads also occur together with soil loss, associated with soil particles carried into the water body.

Normally in modeling studies phosphorus is mechanistically simulated by two forms, soluble (mainly the phosphate) and particulate (organic or particle-associated form), in both the soil and water columns. Accordingly, two major phosphorus pools, labile and stable, are often assumed to exist in the soil content, interact with each other through immobilization and mobilization processes, and determine the available amount of nutrient release. The phosphorus content in either soil pool is determined by land use and soil type and varies with the processes of accumulation and depletion. Manure application and eluviation after rainfall are the two most important external drivers for the variation of soil content.

Phosphorus exists in water also in particulate and dissolved phases. The mechanism of nutrient transformation in water columns is currently still unclear. Uptake and release could occur through biological processes such as plant or bacterial use of the solute, or through abiotic complexation of the solute with suspended particles or those on the streambed. Studies have demonstrated that phosphate is removed quickly from the water column by abiotic processes, and that phosphorus concentration in stream water is held in equilibrium by abiotic exchange (Meyer 1979). Phosphorus uptake is strongly related to the particulate surface area available for phosphate adsorption, which is determined by the abundance of fine detritus or concentration of fine-grained sediments present in the stream (Munn and Meyer 1990; Valett et al. 2002). Uptake is also highly affected by the hydrological characteristics of flow, physical character of stream channels and even riparian conditions (Meyer et al. 1999). Generally, in a river system, the behavior of phosphorus is dominated by abiotic mechanisms such as dispersion, adsorption and desorption of phosphorus to suspended solids, and for a lake or reservoir, the effects of biological processes, such as algal growth and decomposition, are more important.

5.2 The Chattahoochee watershed

5.2.1 Watershed characteristics

For a comprehensive watershed study, a large amount of information needs to be collected and analyzed, to obtain an accurate understanding of the watershed characteristics. The required data from natural, social and economic dimensions include meteorological conditions, land cover types, distribution of residences and major point sources, current and historical water quality conditions, existing pollution control implementations, as well as the future prediction of watershed evolution and developing trends in the surrounding areas. This information is briefly described in the following paragraphs.

The Chattahoochee River flows from the Blue Ridge Mountains in the northwest corner of Georgia, through the metropolitan Atlanta region, along the Georgia-Alabama border, and ends in Lake Seminole at the Georgia-Florida border. The Chattahoochee River Basin is a part of the large Apalachicola, Flint, and Chattahoochee system (ACF), which ultimately discharges to the Gulf of Mexico through the Apalachicola Bay on the Florida panhandle (displayed in Figure 5-2). It is characterized by a warm and humid, temperate climate. Average daily temperatures in the basin are about 7~10 °C for January and 24~27 °C for July. Average annual precipitation in the basin, primarily as rainfall, is about 1400 mm. Actual evapotranspiration (the sum of direct evaporation and transpiration by plants) generally increases from north to south and ranges from about 800~1100 mm.

The metropolitan Atlanta region lies between the Upper and Middle Chattahoochee watershed, respectively USGS HUC codes 03130001 and 01310002. Their location in Georgia and the corresponding terrain map are shown Figure 5-3. In 1990, the Chattahoochee watershed had a population of 2.6 million people; population growth in the watershed was about 20% between 1990 and 1998 (CWI 2000). In this area the metropolitan Atlanta district has had the highest population growth rate in U.S. for the last 20 years. This rapid growth has brought a significant change from forested to urban or developed use of land, required an enlargement in water supply from the already limited surface water resources, and, of greater concern, placed additional environmental stresses by discharging more contaminants into the waterbody and altering the intrinsic behavior pattern of the natural system (Beck et al. 2008b).

There are two main lakes located upstream and downstream of the city of Atlanta. Lake Lanier is upstream and provides the water supply for the metropolitan Atlanta area, while Lake West Point is located downstream and receives the effluent. Since lakes are the most sensitive locations for environmental problems concerning nutrients, we will focus in this study on the impact of the watershed around metro-Atlanta on the water quality response in the receiving waterbody, Lake West Point. Specifically, the study watershed of interest covers the 4,500-km^2 drainage area of the main stem segment of the Chattahoochee River, from Buford Dam at the outflow of Lake Lanier, southwards past the city of Atlanta, as far as the inlet to Lake West Point.

Lake West Point is located 95 kilometers downstream of Atlanta. It is a U.S. Army Corps of Engineers reservoir impounded by the construction of West Point Dam for flood control, hydroelectric power generation, navigation, fishing, wildlife development and general recreational activities. With a drainage area of 8,800 km^2, the reservoir has a surface area of 105 km^2 and storage volume of 746 million m^3. It has an average inflow of 136.6 m^3/s and a discharge of 136.2 m^3/s, as summarized from online monitoring data by U.S. Army Corps of Engineers.

Previous research has shown that the instream concentration and load of nutrient increase by 7-10 times as the river passes through the metropolitan Atlanta region (Frick and Buell 1999). Phosphorus load is the major concern in this watershed since many lakes ini Georgia have recently exhibited signs of nutrient enrichment. This enrichment will result in dense algae growth and lake eutrophication. High nutrient concentrations and ecological degradation have been observed in the summer.

5.2.2 Environmental management issues

The continuing rapid urban development and population growth in this area will inevitably result in an increase on the demand for water resources; furthermore, the pollution discharges will exacerbate problems of water resources and the water environment. As a result, metro Atlanta and its surrounding areas now face three critical water quality problems: storm water runoff that lacks effective control, increasing wastewater effluents form municipal sewage, and district-wide insufficient TMDL planning and implementation (MNGWPD 2003).

Under the NPDES (WPD 2006) over forty point sources are located in this portion of the Chattahoochee watershed. Most of them are municipal wastewater treatment facilities. Their spatial distribution is shown in Figure 5-4. Among them, the R.M. Clayton Water Pollution Control Plant, with a capacity of over 100 million gallons per day (MGD) and treating the municipal wastewater from the downtown Atlanta area, is the largest wastewater treatment plant in the southeast United States. Nonpoint sources are also an important contributor of phosphorus loading in the Chattahoochee watershed. Analysis of water quality data indicates that urban and agricultural lands in the watershed are significant sources of nutrients. In previous research, modeling estimates show that approximately 20% of the phosphorus loading comes from point sources in the portion of HUC 03130001 and 40% in HUC 03130002 (MNGWPD 2003). Another study has shown that point sources discharged 70% of the phosphorus load in the basin above West Point Lake (Emmerth and Bayne 1996).

Since the 1970s, essentially aiming at conserving and improving the water quality and ecological environment of lakes and reservoirs, major improvements in water quality have occurred in the Chattahoochee Basin, as a result of implementing of secondary treatment for all Atlanta-area wastewater treatment facilities (Calhoun et al. 2003; EPA 2000b), despite rapid urban growth during this period. However, these efforts have been directed at improving dissolved oxygen (DO) in the river. For phosphorus, however, the performance of wastewater treatment is quite unsatisfactory. Furthermore, due to the difficulties in monitoring and enforcement of diffuse sources, there are no direct regulations for controlling their nonpoint sources – it is achieved to a limited extent by voluntary programs. Lack of incentives is an important obstacle for nonpoint pollution control and abatement here. In addition, the decreasing stream flow levels induced by the severe drought of the past several years has also led to an increase of nutrient concentrations, and the risk of lake eutrophication.

With respect to ambient water environment management, no national or state standards have hitherto been established for concentrations of phosphorus compounds in water, alrough to control eutrophication the EPA makes the following recommendations: total phosphorus should not exceed 0.05 mg/L in a stream at a point where it enters a lake or reservoir, and should not exceed 0.1 mg/L in streams that do not discharge directly into lakes or reservoirs.

At present, the Chattahoochee watershed does not have a TMDL for phosphorus, but the Georgia Environmental Protection Division has enacted a Watershed Management Plan for the Metropolitan North Georgia Water Planning District and set watershed limits for phosphorus loadings into lakes (MNGWPD 2003), which are listed in the Table 5-1. In association with the data of annual inflow to Lake West Point, which is 4.31×10^9 m^3 calculated from the historical data from 1976 to 2007, we can evaluate the allowable average concentration of total phosphorus in the reservoir inflow based on the EPD's phosphorus load limit, which is calculated as 0.147 mg/L, hence higher than the EPA's recommendations.

5.3 A comprehensive simulation system

As we mentioned in previous chapters, models are used as an important tool for watershed study. Based on the above analysis of the general features of a watershed system, as well as the significant characteristics of the large-scale Chattahoochee Basin, we will construct herein a dynamic watershed simulation system to explore the overall watershed hydrological and pollutant behavior and to make an accurate evaluation of the response of influential factors and instream water quality conditions. This modeling system is the core part of the entire IMUSEM system and will behave as a basis for the further management-supporting task concerning TMDL planning and water quality trading.

A set of models is first assembled into a comprehensive model system so that the nutrient discharges from point and nonpoint sources to a river system and the in-stream routing processes can be simulated in a consistent and compatible manner. This integrated model system comprises three component models, to mimic the fully dynamic behavior of nonpoint source fluxes from a number of sub-basins throughout the entire watershed, discharges from point sources such as wastewater treatment plants, and the subsequent pollutant transport and transformation processes along the river channel. The structure of this model assemblage is quite similar to an integrated watershed model structure we have constructed and successfully tested in previous research (Shi 2004).

Specifically, BASINS-HSPF is applied to estimate pollutant loads from nonpoint sources (each sub-basin), mainly focusing on the precipitation-runoff and associated watershed hydraulic processes. The WEST-based realization of Activated Sludge Model No.2d (ASM 2d) (Henze et al. 1999) simulates the dynamic behavior of the point source, i.e., the treated sewage discharges from urban wastewater treatment plants. The consequences of these nonpoint and point discharges for the water quality response of the receiving river are then simulated by a newly developed model STAND2, upgraded from the model of STAND. The schematic structure of this assembled model system is illustrated in Figure 5-5.

The simulation system has been set up to mimic closely the context of metropolitan Atlanta within the Chattahoochee watershed, such that we can generate all manner of stream water quality as a function of watershed characteristics, polluter impacts, as well as other external and internal forces. In essence, the principal outputs of interest from the model system are the concentrations of suspended sediment and phosphorus at various points along the river system, provided as daily time-series for a variety of hydrological years.

After the entire model assemblage is constructed, it is embedded into a sampling-based framework for model calibration, and then applied for evaluating watershed and water quality conditions, all under uncertainty. Here the available onsite monitoring data series are obtained from the USGS website, with a daily observation for discharge rate and monthly measurements for total phosphorus concentration. Considering the target of this simulation study, for exploring the dynamic behavior of pollutants in the watershed system, our modeling system is operated on a daily basis, these phosphorus monitoring data are considered very sparse indeed. Based on them, the calibration process is mainly directed at the channel processes, in STAND2. For the nonpoint sources and point-source simulation components, the models of HSPF and ASM 2d, their simulations are conducted with the parameters values retrieved from the literature, default values in the model parameter library, and previous research experience. After calibration, the modeling system is subsequently applied to assessing the resulting conditions under various watershed management policies, for evaluating their performance and effectiveness in the presence of (significant) uncertainties.

5.4 Nonpoint source assessment

Watershed nonpoint source releases, mainly caused by the rainfall-runoff process, i.e., precipitation, interception, surface storage and detention, infiltration, surface runoff generation, mobilization and erosion of sediment, and associated phosphorus behavior, are modeled by BASINS/HSPF. BASINS is a multi-purpose environmental analysis system that integrates a GIS, national watershed data, and state-of-the-art environmental assessment and modeling tools into one convenient package (EPA 2008a). It is a widely used software platform to facilitate the examination of environmental information, support the analysis of environmental systems, and provide a framework for examining management alternatives. Version 4.0 was first released in 2007, featuring a new open-source GIS software architecture named MapWindow and several enhancements of the included models.

The most important watershed characteristic that determines nonpoint discharge is the land cover condition, which is retrieved from GIRAS (Geographic Information Retrieval and Analysis System) landuse/landcover spatial data provided by the online database of EPA and displayed in Figure 5-6. From this figure, we see forest land is the major land-use type in this basin, but actually cropland and feedlots, urban and built-up land, despite a relatively small percentage (summarized in Table 5-2) in total area, contribute a higher pollution loading to the stream water.

With the automatic watershed delineation tool of BASINS, and based on the DEM map (shown in Figure 5-3) and map layer of river channels, the entire watershed is delineated into a number of sub-basins, which is shown in Figure 5-4. Relevant data of the watershed, such as spatial distribution of land-use type are overlaid with the sub-basin layer and the land-cover information extracted for serving the computation of HSPF model in each sub-basin. The land cover conditions (for PERLNDS) are classified as five major types in the HSPF model and their distribution in each sub-watershed is listed in Figure 5-2. In Figure 5-2, we see that the 6th, 10th, 11th, and 12th sub-basins have a large portion of urban and built-up lands, where metropolitan Atlanta is located. The 7th, 13th, and 17th sub-basin contain much agricultural lands; for these sub-basins, the nonpoint sources are considered to have a greater potential for reduction.

Meteorological conditions are an important external factor for nonpoint-source discharge. As the most active variable that drives this hydrologic process, not only is total precipitation amount, but also rainfall type, its temporal and its spatial distribution are influential in the process of runoff generation, soil erosivity and pollutant release. The meteorological data are collected from several USGS weather stations within and nearby this watershed, including GA090451 (GA Atlanta Hartsfield international airport), GA093363 (GA Alpharetta), GA092485 (GA Dallas), and GA091640 (GA Carrollton), whose locations are displayed in Figure 5-8.

Using as inputs to this model the meteorological data (annual series at up to an hourly basis), together with topographical and land cover conditions, and associated parameters, corresponding spatial distributions of runoff and nonpoint-source pollutant loadings can then be generated for each individual sub-basin. The model outputs have a lot of information, and we are interested in the flow rate and pollutant yield. Choosing the year of 1995, which was a moderate hydrological year, and the 13^{th} sub-basin (Sweetwater Creek watershed) as an example, the computed phosphorus concentrations and discharge rates are plotted on a daily basis in Figure 5-7.

We have simulated the pollutant load for all the 17 sub-watersheds, for which the time series are not shown in this document. However, we have calculated the annual average (flow-weighted) total phosphorus concentration in runoff for each subbasin, and displayed it in Figure 5-8 to reflect the spatial distribution of nonpoint source pollution in the whole area. In Figure 5-8, we see that the metro Atlanta region releases more nutrients than other suburban and rural areas. In conjunction with the map of land use type distribution (shown in Figure 5-6 and Table 5-3) and current trends of urban development in the Atlanta region (ARC 2003), we may tentatively conclude that the urban runoff (from urban and developed area) contributes more for the total pollutant load than agriculture lands, which are actually normally believed to be primary nonpoint source.

5.5 Point source assessment

The pollutant loads from point sources are evaluated based on NPDES permit and available monitoring data. According to NPDES, there are about forty point source dischargers located in this segment of the Chattahoochee watershed (the total number is higher, but quite a few of them are discontinued or inactive). In Table 5-3 the issued yearly discharge permits are listed, as well as the actual average flow rate and total phosphorus loadings estimated by the environmental authority. The actual discharge and nutrient load monitoring data are only available for 14 major point sources, in upper half of Table 5-3; but for the relatively minor point sources, actual nutrient discharge data are unavailable (lower half of the table)

As stated in the Chattahoochee River Basin Management Plan, all major municipal NPDES facilities between Buford Dam and West Point Lake are required to meet a phosphorus limitation of 0.75 mg/L monthly average. The City of Atlanta water pollution control plants are required to meet a monthly average phosphorus limitation of 0.64 mg/L (GAEPD 2003). The summary of annual nutrient loadings in Table 5-3 shows that all of the major facilities in this stretch of the river are currently complying with these criteria.

Hitherto for a watershed-scale environmental study incorporating both point and nonpoint sources, the point sources are usually evaluated with static functions. However, in the present model system, the behavior of the urban wastewater treatment system is accounted for in a dynamic manner, instead of approximating it as a vector of time-invariant constants. This is a distinctive feature. In the present case study, dynamic simulation of just the single discharge from Atlanta's largest wastewater treatment plant, the R.M. Clayton facility is applied as an illustration. The facility is designed to treat a maximum daily flow of 100 million gallons of wastewater for discharge to the Chattahoochee River under the NPDES Permit. Its high-frequency behavior is simulated within an advanced software platform, WEST (World wide Engine for Simulation, Training and automation). WEST is a user-friendly platform and powerful tool for the modeling and simulation of wastewater treatment plants. It can be used for engineering design and control. From its "library" of model options, Activated Sludge Model No.2d has been selected for our present purposes; it provides simulation of removal of phosphorus (the focal pollutant/nutrient here) by biological and chemical (precipitation) means.

Given previous detailed and comprehensive studies of (simulated) wastewater treatment plant behavior (Jiang 2007; Jiang et al. 2005), patterns of treated sewage discharges to the Chattahoochee River, which are typical for Georgia, can be obtained. Under different representative hydrological conditions (wet, dry and moderate), signaling thus the important fact that our simulation can take into account the impacts of these and other dynamic perturbations, sequences of simulated discharge rates and effluent total phosphorus concentration are produced. For the year of 1995 (a moderate hydrological year), they are as shown in Figure 5-9.

5.6 In-stream simulation

5.6.1 Model development

Our third component in the integrated simulation system for the Chattahoochee watershed is the river simulation module, the model of STAND2. This model is actually a part (river component) of the WWQS (Watershed Water Quality Simulator) system (Shi and Beck 2008). The instream hydraulic, sediment, and phosphorus behaviors in the main stem of the Chattahoochee river are simulated by this model.

STAND2 has recently been developed from the original version of STAND, which is an innovative model and has been applied in several case studies with good performances in simulating the dynamic hydrological, sediment and nutrients behavior in streams (Zeng 2001; Zeng and Beck 2001). Compared with the former version written in C++, this new Visual Basic version has incorporated several upgrades, including computational optimization, many minor revisions of equation forms and parameters, and new tools to study phosphorus in both soluble and insoluble forms instead of only the orthophosphate form, (as previously).

STAND2 has inherited the three-layer linked structure of STAND and some other good steam water quality models such as QUAL2EU (EPA 1990). The flow, sediment and pollutant routing in the stream are simulated by this model. All the internal process are described with partial differential equations and the continuity equation is solved with a finite difference approximation using a forward explicit scheme for achieving numerical integration. Next, we will introduce included parts and functions in the model structure. In detail, the structure and components of STAND2 are as now described.

5.6.2 Hydraulic simulation

In the stream hydraulic component, we take the assumption of a trapezoidal channel cross-section and use the equations in the conventional de Saint-Venant methods in conjunction with Manning's equation to account for the hydraulics of open-channel flow. The unsteady flow in the open-channel is expressed with the following equation:

$$\frac{\partial A}{\partial t}+\frac{\partial Q}{\partial x}-q_l=0 \qquad (5\text{-}1)$$

where A is the wetted cross-section area (m^2); Q is the cross-section averaged discharge (m^3/s); q_l is the rate of lateral inflow (m^2/s), which is generated by the two other component models; x is the spatial coordinate, longitudinal along the reach (m); t is the temporal coordinate (s).

The other important equation used here is Manning's equation, which describes the relationship between the discharge and stream stage, as

$$Q=\frac{1}{n}\cdot A\cdot R_h^{\frac{2}{3}}\cdot s^{\frac{1}{2}} \qquad (5\text{-}2)$$

where n is Manning's coefficient of roughness, which determines the hydraulic conductivity of the channel and behaves as another very sensitive parameter here; R_h is hydraulic radius (m); s is the energy slope. R_h is calculated by

$$R_h=\frac{A}{wetP} \qquad (5\text{-}3)$$

where $wetP$ is the wet perimeter at the cross section (m).

In the simulation of the unsteady channel flow, we solve this partial differential equation by a numerical integration algorithm. The de Saint-Venant equation is subject to initial and boundary conditions. We set the initial condition to be consistent with the in-site measurements at the start time point $Q(x,0)$. The upper boundary condition is set as the time series of upstream inflow rate into this river segment $Q(0,t)$. Normally two forms of lower boundary conditions are employed, the time series of water stage at the downstream boundary or the assumed stage-discharge relationships. Here we choose the latter form, which is actually expressed through Manning's equation.

We apply the explicit finite difference scheme for the discretization and solving the difference equations by the iterative approach of numerical integration. The discretized form is

$$A_i^{j+1} = A_i^j - \frac{\Delta t}{\Delta x}\left(Q_i^j - Q_{i-1}^j\right) + q_l \cdot \Delta t \qquad (5\text{-}4)$$

Where j is the temporal step; i is the spatial step. Δt (s) and Δx (m) are the respective step lengths.

Jointly applying the above equation and the stream discharge-stage relation, we can calculate the stream flow at $t+\Delta t$ based on the known current condition:

$$Q_{t+\Delta t} = F_{Forward}\left(Q_t, \Delta t\right) \qquad (5\text{-}5)$$

where $F_{Forward}$ represents the combination function of the two relevent equations. Moreover, in order to control the error generated by the numerical integration process and assure the convergence of this algorithm, we employed a step-adjusting procedure to find the optimal time step. For each one step of Δt, we calculate the condition after one whole step by the above equation, and at the same time, we calculate the conditions after two half-steps with the forward equations, expressed as

$$Q'_{t+\Delta t} = F_{Forward}\left(F_{Forward}\left(Q_t, \Delta t/2\right), \Delta t/2\right) \qquad (5\text{-}6)$$

If the difference between these two calculations is small enough: $\left|Q_{t+\Delta t} - Q'_{t+\Delta t}\right| < e$, we accept the results and continue to next time step, or else we will decrease the step length and compute again. By this means, at least the first-order error will be confined to be lower than a threshold. This step-varying algorithm is also employed for the simulation of sediment and nutrient behavior.

5.6.3 Sediment transport component

For simulation of the in-channel behavior of suspended solids, we take into account the processes of advection, dispersion, deposition and channel erosion. The sediment transport component computes sediment transport potential (flow carrying capacity) and actual transport rates based on hydrological behavior. The suspended sediment in the stream flow is evaluated by the advection-dispersion equation of

$$\frac{\partial(A \cdot C_s)}{\partial t} + \frac{\partial(Q \cdot C_s)}{\partial x} = \frac{\partial}{\partial x}\left(A \cdot E_s \cdot \frac{\partial C_s}{\partial x}\right) + C_{s\_Lat} \cdot q_l + A \cdot P_s \qquad \text{(5-7)}$$

The discrete form of this partial differential equation is:

$$\begin{aligned} A_i^{j+1} C_i^{j+1} &= A_i^j C_i^j - \frac{dt}{dx}\left(Q_i^j C_i^j - Q_{i-1}^j C_{i-1}^j\right) \\ &+ \frac{dt \cdot E_s}{dx^2}\left(A_i^j C_{i+1}^j - A_i^j C_i^j - A_{i-1}^j C_i^j + A_{i-1}^j C_{i-1}^j\right) + C_{s\_Lat} \cdot q_l \cdot dt + A_i^j \cdot P_s \cdot dt \end{aligned} \qquad \text{(5-8)}$$

where C_s is the concentration for suspended solid (mg/L); E_s is the dispersion coefficient (m^2/s); C_{S_Lat} is the concentration in lateral inflow; P_s is the sediment source/sink term due to the process of deposition/scouring (mg/L/s).

Similar to the computational method employed in the previous section for hydraulic simulation, we use the explicit finite difference algorithm for the numerical integration. The in-channel source/sink term is determined by the rate of scouring and deposition. The flow carrying capacity is an important item in this calculation. We take the assumption that, if the steam suspended solid concentration is larger than the carrying capacity, net deposition will happen, otherwise the entrainment or scouring will be the dominating process. The source/sink term has the effect that the in-stream concentration of suspended solids approaches the carrying capacity. We use a first order mechanism to describe it

$$P_s = k_{sed}\left(C* - C_s\right) \qquad (5\text{-}9)$$

where k_{sed} is the coefficient that describes the rate as which the actual suspended sediment concentration approaches its potential (1/s); $C*$ is the suspended sediment carrying capacity (mg/L);

In STAND the sediment transport potential is calculated with a unit stream power-law approach, with a very complex empirical equation (Yang 1996). But in this model, we use a more simplified equation, which is

$$C_* = r_{sc}\left(\frac{V^3}{gR_h\omega}\right)^{k_{sc}} \qquad (5\text{-}10)$$

In this equation, V is the average stream flow velocity (m/s), r_{sc} and k_{sc} are the coefficient and index; and ω is the settling velocity for sediment particles (m/s). Sediment falling velocity ω is calculated according to the following hydro-mechanical equations (Van Rijn 1984)

$$\omega = \begin{cases} \dfrac{(\tau - 1.0) g d_s^2}{18\upsilon} \quad if\ (d_s < 10^{-4}) \\ 1.1\left((\tau - 1.0) g d_s\right)^{\frac{1}{2}} \quad if\ (10^{-4} < d_s < 10^{-3}) \\ \dfrac{10\upsilon}{d_s}\left(\left(1.0 + \dfrac{0.01(\tau - 1.0) g d_s^3}{\upsilon^2}\right)^{\frac{1}{2}} - 1.0\right) \quad if\ (d > 10^{-3}) \end{cases} \qquad (5\text{-}11)$$

where τ is the specific gravity of sediments (2.65 for quartz while 1.0 for water); υ is the kinematic viscosity (m^2/s), ($1.03\times10^{-6}\ m^2s^{-1}$ for water at 20°C); d_s is the representative particle dimension (m); and g is the constant of gravitational acceleration (m/s^2).

In the assumptions, k_{sed} has different expressions when deposition or entrainment dominates. When net deposition occurs, for each small compartment (for composing the one-dimension channel) in the discrete form and through a single time step dt, the sediment deposition is calculated as

$$P_s \cdot A \cdot dx \cdot dt = \frac{\omega \cdot dt}{Dep} \cdot (C_* - C_s) \cdot A \cdot dx \qquad (5\text{-}12)$$

Based on this equation, we have

$$P_s = \frac{\omega}{Dep} \cdot (C_* - C_s) \qquad (5\text{-}13)$$

and $k_{sed} = \dfrac{\omega}{Dep}$ (5-14)

where Dep is the current average depth in this cross section (m).

For cases where actual sediment concentration is lower than the flow carrying capacity, the process of channel scouring or bed sediment entrainment is likely dominating. Then the source item is calculated with

$$P_s \cdot A \cdot dx \cdot dt = Ent \cdot wetP \cdot dx \cdot dt \qquad (5\text{-}15)$$

and $P_s = \dfrac{Ent}{R_h}$ (5-16)

Here *Ent* is the channel scouring intensity ($ML^{-2}T^{-1}$), calculated by

$$Ent = k_{ent} \cdot s \cdot \frac{(V - V_{cr})}{V_{cr}} \qquad (5\text{-}17)$$

where k_{ent} is the erodibility coefficient or sediment entrainment coefficient ($ML^{-2}T^{-1}$); V_{cr} is the critical velocity for sediment entrainment (LT^{-1}). V_{cr} is calculated with

$$V_{cr} = \begin{cases} 2.05\omega \quad if\ (U_* \geq 70\upsilon) \\ \left(\dfrac{2.5}{\log_{10}\left(\dfrac{U_* \cdot d_s}{\upsilon}\right) - 0.06} + 0.66 \right) \cdot \omega \quad if\ (U_* < 70\upsilon) \end{cases} \qquad (5\text{-}18)$$

where U^* is the shear velocity (m/s). It is obtained by

$$U_* = (gR_h s)^{\frac{1}{2}} \qquad (5\text{-}19)$$

Therefore, the source/sink term when scouring dominates is expressed by

$$P_s = k_{ent} \cdot \frac{s}{R_h} \cdot \frac{(V - V_{cr})}{V_{cr}} \qquad (5\text{-}20)$$

5.6.4 Morphological adjustment of bed

The bed morphological adjustment is simulated in this model, with the equation of

$$\frac{dA_s}{dt} = \frac{d}{dt}\left(\frac{P_s \cdot dt \cdot A \cdot dL}{\lambda \cdot \rho_{Sed} \cdot dL}\right) = \frac{A \cdot P_s}{\lambda \cdot \rho_{Sed}} \qquad (5\text{-}21)$$

where dA_s is the change of cross section area due to the sediment deposition or scouring; ρ_{sed} is the dry density of bed sediments (g/m^3), and λ is the porosity of bed sediments. We assume that the shape of the channel profile does not change with morphological change happens, so that we have

$$dA_s = -d(elevation \cdot wetP) \qquad (5\text{-}22)$$

Then we can estimate the channel bed and bank adjustment during the simulation period with the equation of

$$\frac{d(elevation)}{dt} = -\frac{A \cdot P_s}{\lambda \cdot \rho_{Sed} \cdot wetP} \qquad (5\text{-}23)$$

where *elevation* is the elevation of cross sections along the stream (m).

5.6.5 Water quality component

Phosphorus exists in water in both particulate and dissolved phases. Here the in-stream phosphorus is simulated as *SP* and *AP*. *SP* is the dissolved form, mostly inorganic, very reactive, and orthophosphate accounts for the majority of it. *AP* is the sediment-associated phosphorus, which is the phosphorus tightly bound to the suspended sediment particles. *AP* is the relatively stable form in water, including both inorganic and organic forms.

The behavior of phosphorus in stream water is a complicated problem governed by several physical, chemical and biological processes such as adsorption and desorption to the sediment, immobilization and mineralization between inorganic and organic forms, bio-uptake by vegetation, internal and external source release, and so on. Based on preceding discussion and relevant research experience, the main in-stream phosphorus transformation process in this model is expressed as the adsorption and desorption associated with suspended solids. The behaviors of phosphorus and sediment are displayed in Figure 5-10.

The concentration of dissolved phosphorus is simulated by the following partial differential equation:

$$\frac{\partial(A \cdot C_p)}{\partial t} + \frac{\partial(Q \cdot C_p)}{\partial x} = \frac{\partial}{\partial x}\left(A \cdot E_p \cdot \frac{\partial C_s}{\partial x}\right) + C_{p\_Lat} \cdot q_l + A \cdot P_p \qquad (5\text{-}24)$$

which has a discrete form of

$$\begin{aligned} A_i^{j+1} C_i^{j+1} &= A_i^j C_i^j - \frac{dt}{dx}\left(Q_i^j C_i^j - Q_{i-1}^j C_{i-1}^j\right) \\ &+ \frac{dt \cdot E_p}{dx^2}\left(A_i^j C_{i+1}^j - A_i^j C_i^j - A_{i-1}^j C_i^j + A_{i-1}^j C_{i-1}^j\right) + C_{p\_Lat} \cdot q_l \cdot dt + A_i^j \cdot P_p \cdot dt \end{aligned} \qquad (5\text{-}25)$$

where C_P is the concentration of the dissolved phosphorus component of interest (mg/L); E_P is the dispersion coefficient (m^2/s); P_P is a source/sink term (mg/L/s); and C_{P_Lat} is the phosphorus concentration in lateral inflow (mg/L).

The change of phosphate concentration in the stream is represented by P_P. The calculation of P_P takes into account the transformation between different forms of phosphorus, through adsorption and desorption of dissolved phosphorus to suspended sediment in this model. In existing models such as STAND or HSPF, first-order kinetics or a Freundlich equation are often used to account for these processes. In this model, we compared these two process and adopted the assumption of an equilibrium process, which shows the concentration of dissolved form of phosphorus is approaching to the equilibrium concentration with a certain sorption rate,

$$P_p = k_{Phos} \cdot \left(C_p - C_{eq}\right) \qquad (5\text{-}26)$$

Here k_{phos} is the phosphate adsorption coefficient (T^{-1}); and C_{eq} is the equilibrium concentration of dissolved phosphate (mg/L), which is considered as a function of the amount of total phosphorus and suspended sediment concentration.

We use the following adsorption equation to estimate the equilibrium concentration. Under the equilibrium condition, the adsorption equation can be expressed as

$$r_{attached} = k_{pf} \cdot C_{eq}^{\beta} \qquad (5\text{-}27)$$

where $r_{attached}$ is the total amount of phosphorus in the adsorbed phase; β is the empirical constant that provides an estimate of the intensity of sorption, for which we choose its maximum value of 1 instead of using a varied parameter here; k_{pf} is the Freundlich adsorption constant. Then the soluble phosphorus (orthophosphate) concentration is calculated by the following equation:

$$C_{eq} = \frac{C_{TP}}{1 + k_{pf} \cdot C_s} \qquad (5\text{-}28)$$

The concentration of solute adsorbed to the solids is calculated by

$$C_{PA} = C_s \cdot r_{attached} \qquad (5\text{-}29)$$

According to the mass conservation we have

$$C_{TP} = C_{PA} + C_{eq} = C_s \cdot k_{pf} \cdot C_{eq} + C_{eq} \qquad (5\text{-}30)$$

5.6.6 Model deployment

The simulated watershed system addresses the river segment between Lake Lanier and Lake West Point and the associated drainage area. With information obtained through investigation and pior computational results, we are able to deploy STAND2. For this part of stream hydrological and water quality simulation, the series of daily discharges from Buford Dam, which is the upstream inflow into the smulated river segment, are taken as the upper boundary condition. The data on discharge rate and total phosphorus concentration come from observations at two USGS gages, 02334400 and 02334430, located in Lake Lanier and on the Chattahoochee River at Buford Dam.

Together with the upstream flow, the nonpoint-source and point-source pollutant loads generated by their respective sub-models collectively provide the external forcing functions for the stream simulation. In accordance with the watershed delineation of sub-basins, the river channel of the main stem of the Chattahoochee between Lanier and West Point is divided into 13 segments, by cross sections located at the outlet of each sub-basin (shown in Figures 5-4 and 5-8), the nonpoint- and point-source releases from each sub-basin contribute to the corresponding channels as lateral inflow. The river model behaves, therefore, as a connection between each subbasin discharge, for achieving an overall comprehensive simulation structure, as shown in Figure 5-11.

The topographical data used in this model include the location and elevation of each cross section and the average channel slope. They are all extracted from the DEM map. The elevation profile along the river channel is displayed in Figure 5-12. In this model, we assume cross sections have the shape of a trapezoid. The area of a cross section can be easily calculated with information on the width of the bottom, side slope and depth. In order to conduct the computation of numerical integration, each channel segment is further discretized into several connective compartments. We initialize the conditions of each compartment through a process of linear interpolation.

5.7 Model calibration

5.7.1 Observed data series

The first task after model development is to reconcile our model with the on-site measurements. The in-stream processes are characterized here by a set of parameters (coefficients) associated with the fluvial characteristics. For this first-time application of STAND2 to the Chattahoochee River, the value of these parameters should be obtained by the process of calibration. Since this research focuses on the impacts of a metropolitan watershed on the downstream lake system, we are highly interested in the discharge rate and total phosphorus concentration at the inlet to Lake West Point. The inlet is close to USGS station 03328550, at Franklin, Georgia. Choosing 1995 as an example, we have obtained the observation at the USGS gage station for the model calibration, displayed in Figure 5-13. Annual sequences of day-to-day variations in stream water quality are the outputs of our primary interest from the entire simulation system. These monitoring data (for flow and phosphorus concentration) will be used in comparison with the series of simulated results at that location for determining relevant parameter values.

When we examine the shape of the graphed data for the monthly observations of total phosphorus concentration for the year of 1995, two measurements obtained on March 1st (0.35 mg/L) and August 9th (0.24 mg/L) are much higher than other values. The concentration of nutrients in stream water is often highly related with discharge rate. For this case, however, we find no such correlation for explaining the relatively high values of total phosphorus concentration. Especially for the data on March 1st, 1995, the total phosphorus concentration in stream water is even higher than the average concentration in the effluent of the wastewater treatment plant. Thus we doubt that these two points are generated by monitoring error and, therefore, we will conduct a preliminary calculation to check if they should be considered as outliers. An outlier is an observation that lies an abnormal distance from other values in a sample from a population. Here we will use a method of Box Plots for identifying outliers (NIST 2006).

The box plot uses the median and the lower and upper quartiles (defined as the 25th and 75th percentiles). If the lower quartile is Q_1 and the upper quartile is Q_2, then the difference (Q_2 - Q_1) is called the interquartile range or λ. The following quantities (called fences) are needed for identifying extreme values in the tails of the distribution: inner fence ($Q_1 - 1.5\lambda$, $Q_2 + 1.5\lambda$) and outer fence ($Q_1 - 3\lambda$, $Q_2 + 3\lambda$). A point beyond an inner fence on either side is considered a mild outlier. A point beyond an outer fence is considered an extreme outlier. For the data series of total phosphorus concentration, the data on March 1st and August 9th are both outside of the calculated outer fence (-0.045, 0.235), so that we shall consider that these two points are extreme outliers and will not be used for model calibration.

5.7.2 Using RSA approach for calibration under uncertainty

In Figure 5-13 we see that the available monitoring data for phosphorus concentration is very sparse. As a result, it will be hard for us to evaluate the dynamic nutrient behavior based on these data. In many cases, the crux of the problem of a lack of model identifiability, or over-parameterization, is that what one would like to know about the internal description of the system is of a substantially higher order than that which can be observed of its external description (Beck 2002). The problem of data-scarcity will definitely bring extra difficulties and hamper the effectiveness of model identification and the reliability of the subsequent prediction process. It is particularly necessary to address the problem of uncertainty. Therefore the following calibration exercise is the first step of the cradle-to-grave analysis of uncertainty In addition, the RSA approach is particularly suitable for applications to data-scarcity conditions. Indeed, that was precisely the origin of its invention.

The procedure is as follow. Parameters are randomly sampled from their prior parametric spaces (with a rather wide range) and substituted into the model in order to generate model outputs for evaluation. We then conduct the binary classification, based on the behavior definition(as discussed in Chapter 4). Here, when the time series of model output lies within a defined "close vicinity" of the observations, we accept that model run and parameterization as valid system behavior, otherwise not. The corresponding parameter vector is classified into the behavioral set, which is regarded as the posterior parametric distribution. Then each Monte Carlo simulation associated with a parameter vector is classified as exhibiting either behavior or nonbehavior, according to whether the resulting model output falls within the predefined constraints. The behavioral parameter vectors are accepted as the calibration results. Furthermore, the sensitivity of each single parameter is thereby revealed.

RSA is applied here for the task of model calibration under uncertainty. Traditionally, in environmental modeling, parameter calibration works for minimizing the model fitting error to find the "best" or "optimal" parameter set. However, the model's parameter is not always converging to a single point because of a lack of model identifiability. Thus in contrast with the traditional model calibration method, the new feature of RSA application is that the calibration result is not a single parameter vector; instead, it is a posterior distribution of possible values of parameters. More influential parameters will be more accurately identified in this framework.

After this, the calibrated model can be used for watershed assessments, as a basis for further management-oriented studies.

5.7.3 Sampling process

When we employ the approach of RSA for model calibration, the theoretically ideal condition is that we sample on rather broad parametric ranges (all physically rational values), substitute them into the model, and screen out those giving behavioral simulations. However, such as approach is not realistic because of the huge amount of computational work required. Therefore, in this study, to begin we will define a prior parametric range for this model. The most important 7 parameters used in this case are listed in Table 5-4, together with the predefined lower and upper bounds for each parameter, the range between which will later be taken as the "prior parametric distribution" for subsequent RSA applications.

After we determine the range for each parameter, we randomly sample 1000 points with an assumed uniform distribution between the lower and upper bound, obtain a (1000×7) parametric matrix, then run the model with these parameter values, and generate the set of model results - each simulation outputs 365-day time series.

5.7.4 Definition of acceptance threshold

We are simulating and calibrating the model simultaneously on discharge and phosphorus concentration. Fortunately, one significant advantage of the RSA approach here is the convenience of multi-objective computation. In essence, we only need to choose a set of acceptance criteria for each simulated constituent, that is, define the acceptable system behavior for instream discharges, and phosphorus respectively, and employ them as the constraints to screen the behavioral simulations from those nonbehavioral ones.

In order to track how well the model is simulating the real natural system, we will define a measure for evaluating model performance. Four types of indices can be employed as statistical criteria for the definition of acceptance threshold. All of them embody the concept of "acceptable closeness to a set of uncertain process observations" (Chen 1993), which is exactly the purpose of model calibration. In the subsequent computation, an index of the Nash-Sutcliffe (NS) model efficiency coefficient is employed. The NS coefficient is an often-used tool to assess the predictive power of hydrological models, well suited to the present case regarding the large variations associated with transient events. It is defined as

$$NS_i = 1 - \frac{\sum_{t=1}^{T}\left(\hat{Y}_{i,t} - Y_{i,t}\right)^2}{\sum_{t=1}^{T}\left(Y_{i,t} - \frac{1}{T}\sum_{t=1}^{T} Y_{i,t}\right)^2} \qquad (5\text{-}31)$$

where $\hat{Y}_{i,t}$ and $Y_{i,t}$ are the model output and observed data for the i^{th} simulated constituent (flow, TP) at time t (1 to 365 days); T is the total time span to be simulated.

In environmental modeling, the question of "how good a fitting is goodenough" is frequently asked. There is not a general criterion for determining the required extent of fitness, so we may need to determine this for each individual case of model application. In this study, we use a rather flexible approach to determine the acceptance threshold, as follows. Following the model runs with the randomly sampled parameter values, for each simulated constituent a certain portion

(40% in this study) with relatively high NS values are considered the acceptable results. However, because we are simulating multiple state variables simultaneously, a simulation which generates the results meeting the threshold for ALL the simulated constituents is regarded as behavioral simulation. Here we defined a rather broad (loose) acceptable criterion for this case,

$$\begin{cases} NS_{flow} > 0.6 \\ NS_{TP} > 0.3 \end{cases} \qquad (5\text{-}32)$$

In this event, 207 of the total 1000 model simulations are classified as behavioral simulations by the constraints defined above. The empirical joint distribution of these 207 parameter vectors will be taken as the posterior distribution, and the calibration result.

5.7.5 Parametric sensitivity

More significantly, the computation in the RSA allows assessment of the significance of the model's constituent processes and factors to be conducted in terms of criteria of fitness of the model's performance to the observed behavior. The RSA approach generates the K-S statistics of *d* and *Z* index to show the significance of each individual parameter in discriminating between whether an acceptable match to the observations is generated or not. The computation result is listed in Table 5-5. In addition, since these parameters are the surrogates of the processes in the real system, we see that some processes play more important roles than others for enabling model output to fit the observations.

In Table 5-5 we see some parameters have higher impacts under the current simulation framework. If we choose a significance level of 1%, which has a critical value of 1.52 for the two-sample K-S test (listed in Table 4-1), we consider that three parameters are most important. We place them into the Class A. Then we choose 1.07 as the second threshold, which is corresponding to the significance level of 10%, whereby three more parameters are classified into Class B, as less important. The remaining fourteen parameters are found to be not very significant for the current computation, at least when assessed on this univariate basis.

In fact, two factors jointly determine the significance of a parameter in this algorithm: 1) the parameter must be structurally influential; 2) there is high uncertainty (relatively wider range) in the determination of the prior parameter distribution. For those more significant parameters, the uncertainty can be better identified and greatly reduced through the process of RSA, while for those insignificant ones, since the prior and posterior distributions show relatively similar patterns, it follows that there is less potential their associated uncertainty to be reduced.

5.7.6 Simulation results under uncertainty

Through this model calibration process, the computational procedures have achieved two goals. The first goal is to change the values of the model's parameter estimates in order to obtain acceptable, if not best, matches of model-estimated and observed behavior of flow and water quality in the watershed. A second goal, in addition, will be to obtain estimates of the remaining uncertainty (or, conversely, levels of confidence) associated with the model's revised parameter estimates, after calibration.

Running the model with the accepted parameter values, have we generated the results for stream discharge and phosphorus concentration, with uncertainty included. These results are displayed in the Figure 5-14. The red curves are the upper and lower bounds of acceptable (behavioral) simulations, while the green dots are the observed data points. By this means, the uncertainty due to the insufficient reconciliation of simulations and monitoring data are evaluated.

We consider the simulated results shown in Figure 5-14 shows that the model has well captured major trend on the system behavior when we remove the outlying points. So far, we have developed a dynamic model to simulate the watershed hydrological and pollutant behavior and applied the model to a large watershed. The combination of model structure and parameter values represents our understanding on the watershed system. We use this approach and the specific application case to show how the uncertainty can be processed throughout the environmental model development and applications. We hope this framework can be a useful paradigm of modeling-under-uncertainty research in the field of environmental system analysis.

With the simulation model thus set up to mimic the context of metropolitan Atlanta in the Chattahoochee watershed, we can gain more acquaintance on the watershed and pollutant characteristics, and build a technical basis for exploring the uncertainties, and provide substantial benifits for the grand target of underpinning the decision-making process for the scientific watershed and water quality management.

Table 5-1: Phosphorus load limit for Georgia lakes

Lake	Lanier	West Point
Phosphorus load limit (lbs/acre-ft-yr)	0.25	2.4
Phosphorus load limit (lbs/yr)	39,600	1,400,000
Phosphorus load limit (tonne/yr)	18	635
Inflow (m^3/s)	50.7	136.6
Inflow (m^3/yr)	1.6×10^9	4.31×10^9
TP concentration limit (mg/L)	0.011	0.147

Table 5-2: Land use type proportions in sub-basins

Subbasin	Urban and built-up	Agricultural land	Forest land	Wetland and water	Barren land	Area (km^2)
1	6.1%	3.5%	89.0%	0.3%	1.1%	43.6
2	1.3%	15.8%	81.7%	0.0%	1.2%	119.2
3	11.5%	15.6%	72.8%	0.1%	0.0%	139.8
4	10.9%	24.4%	59.7%	0.8%	4.2%	47.3
5	6.5%	14.9%	75.8%	0.4%	2.5%	97.6
6	30.1%	1.8%	62.0%	0.9%	5.2%	57.8
7	7.1%	26.5%	65.1%	0.1%	1.2%	264.3
8	9.2%	7.3%	78.4%	2.5%	2.6%	77.3
9	43.0%	4.9%	44.6%	0.3%	7.1%	120.9
10	56.8%	2.0%	36.9%	0.4%	4.0%	105.2
11	82.6%	0.7%	15.3%	0.3%	1.1%	334.3
12	54.9%	2.6%	37.6%	1.9%	3.0%	319.2
13	14.5%	23.4%	59.7%	0.6%	1.8%	692.5
14	17.7%	9.5%	68.9%	1.1%	2.9%	312.1
15	9.8%	13.8%	72.3%	0.9%	3.3%	725.9
16	1.2%	17.2%	80.3%	0.6%	0.7%	425.5
17	3.7%	21.8%	72.9%	0.3%	1.4%	663.4
Total	19.7%	14.8%	62.7%	0.7%	2.1%	4545.7

Table 5-3: Point sources in the studied Chattahoochee watershed

Name	Permitted flow (mgd)	Avg. flow (mgd)	TP load (lbs/yr)	Avg. conc. mg/L
ATLANTA R.M. CLAYTON WPCP	100	77.8	65228	0.28
ATLANTA SOUTH RIVERR WRC	43.3	33.1	37504	0.37
ATLANTA UTOY CREEK WRC	40	26.5	16392	0.20
COBB CO-SUTTON WPCP	40	31.5	30753	0.32
GWINNETT CO CROOKED WPCP	36	22.9	16966	0.24
COBB CO.-SO. COBB WPCP	28	23.0	31831	0.45
FULTON CO-BIG CREEK WPCP	24	19.8	30172	0.50
FULTON CO-CAMP CREEK WPCP	13	11.3	14484	0.42
FULTON CO-JOHNS CREEK WPCP	7	7.0	11571	0.54
DOUGLASVILLE SOUTH WPCP	3.25	2.3	2576	0.37
NEWNAN WAHOO WPCP	3	1.5		
DOUGLASVILLE (SWEETWATER)	3	1.0	1155	0.37
USAF (LOCKHEED AF PLT No.6)	2.8	2.1	4148	0.64
BUFORD SOUTHSIDE WPCP	2	0.9	1735	0.63
CUMMING WPCP	2	0.9	563	0.20
PALMETTO WPCP	0.6			
DOUGLASVILLE NORTH WPCP	0.6			
VILLA RICA (NORTH WPCP)	0.52			
NEWNAM (SNAKE CREEK WPCP)	0.4			
UNION CITY WPCP	0.25			
BUFORD WESTSIDE WPCP	0.25			
FAIRBURN-LINE CR WPCP	0.22			
FRANKLIN WPCP	0.16			
CARROLL CO-FAIRFIELD WPCP	0.15			
COWETA CO. (ARNCO WPCP)	0.1			
FULTON CO - LITTLE BEAR CRK.	0.1			
DOUGLAS CO BEAVER EST WPCP	0.08			
COWETA CO. (ARNALL WPCP)	0.06			
PINE LAKE MOBILE HOME PRK	0.05			
DOUGLAS (REBEL TRAILS WPCP)	0.04			
FULTON CO-STUBBS RD WPCP	0.037			
DOT REST AREA NO.76 SUWANEE	0.035			
CEDAR HEIGHTS MHP	0.033			
COBB CO - ELMWOOD POND	0.02			
EVOLINE C WEST ELEM SCH	0.009			
COBB CO-ROLLINS WPCP	0.005			
DOUGLAS CO. BOARD ED	0.004			
SUM	351.07			

Data Source: (EPA 2005)

Table 5-4: Parameters and sampling range

Parameter description	Symbol	Lower Bound	Upper Bound	Units
Manning's roughness coefficient	*rfness*	0.02	0.06	--
sediment entrainment coefficient	k_{ent}	0.2	0.5	--
representative particle dimension	d_{sed}	0.05	0.5	mm
SS dispersion coefficient	E_{ss}	50	100	m^2/s
phosphate adsorption coefficient	k_{Phos}	0.04	0.1	1/hr
phosphate equilibrium coefficient	k_{pf}	0.05	0.1	L/mg
phosphate dispersion coefficient	E_p	100	200	m^2/s

Table 5-5: Parameters and sampling range

Parameter	*d*	*Z*	Rank	Class
rfness	0.255	3.273	1	A
k_{ent}	0.070	0.892	6	C
d_{sed}	0.160	2.051	2	A
E_{ss}	0.051	0.654	7	C
k_{Phos}	0.135	1.733	3	A
k_{pf}	0.095	1.214	4	B
E_p	0.082	1.047	5	C

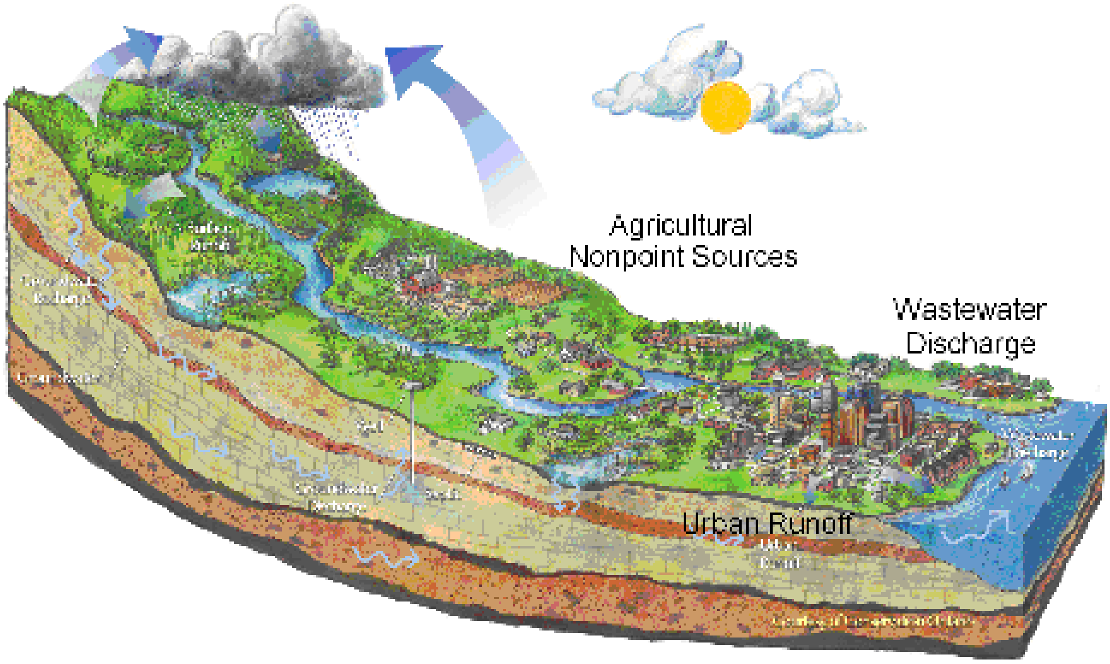


Figure 5-1: Watershed system and pollution sources

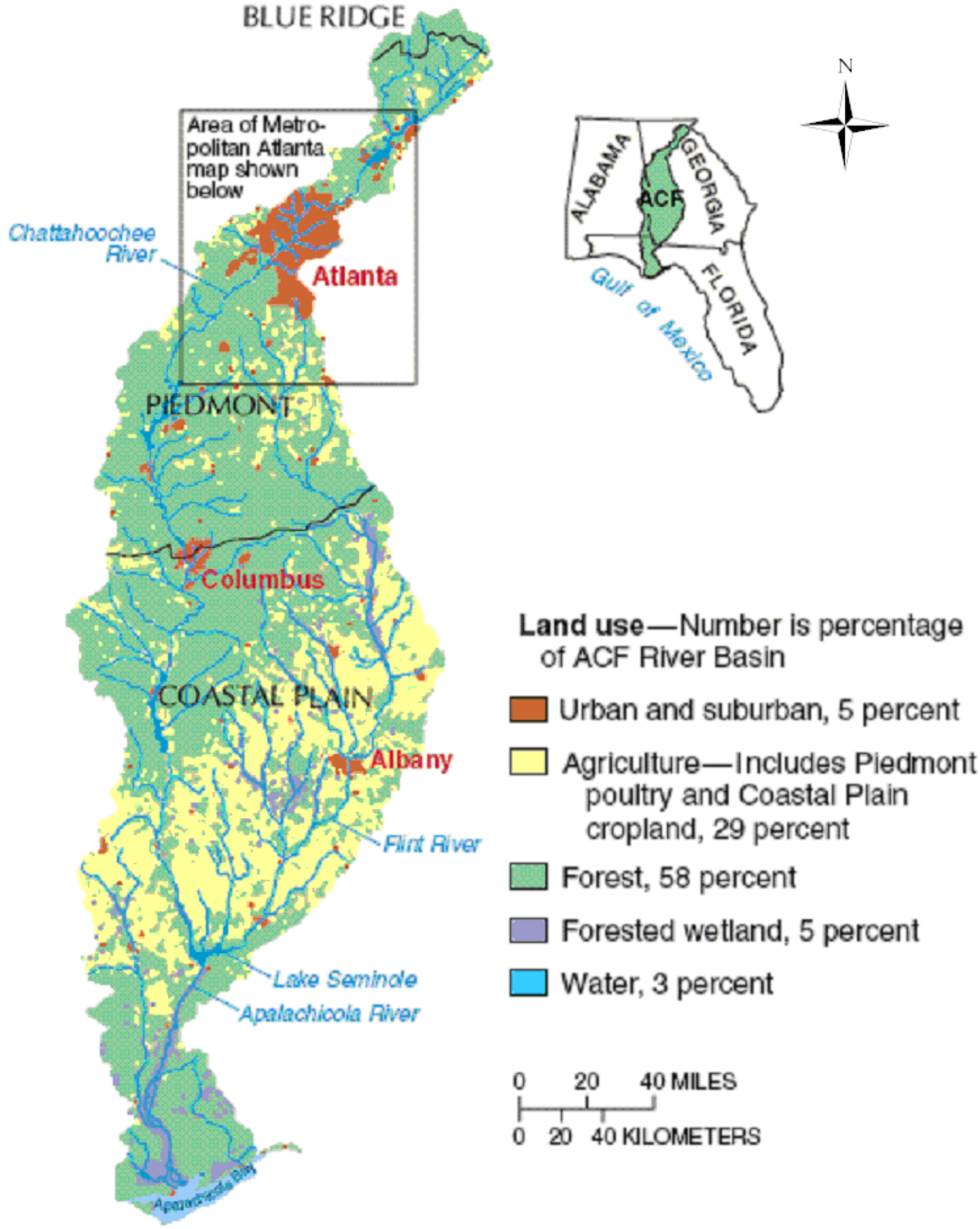


Figure 5-2: Location of Chattahoochee watershed

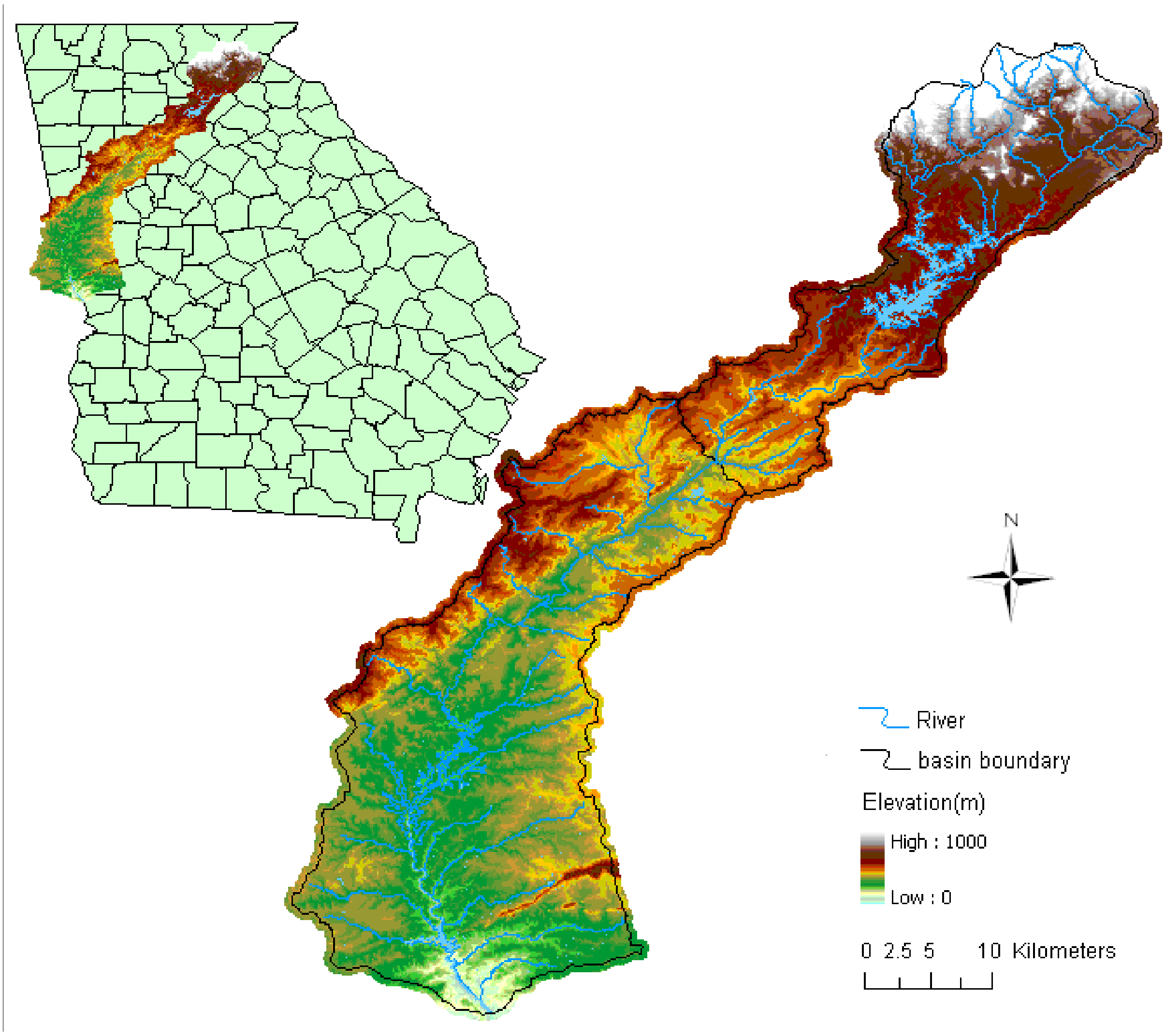


Figure 5-3: Watershed DEM map

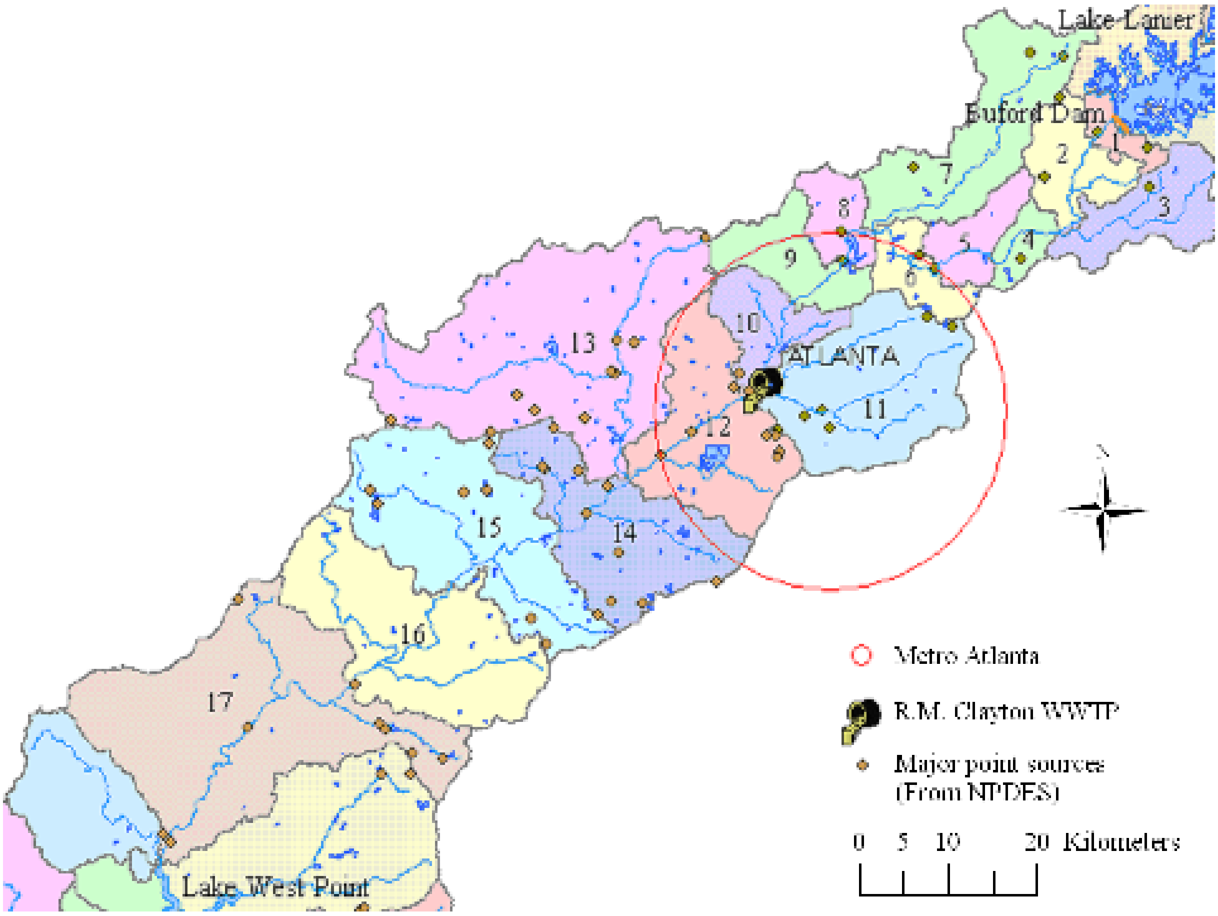


Figure 5-4: Study area and pollution sources

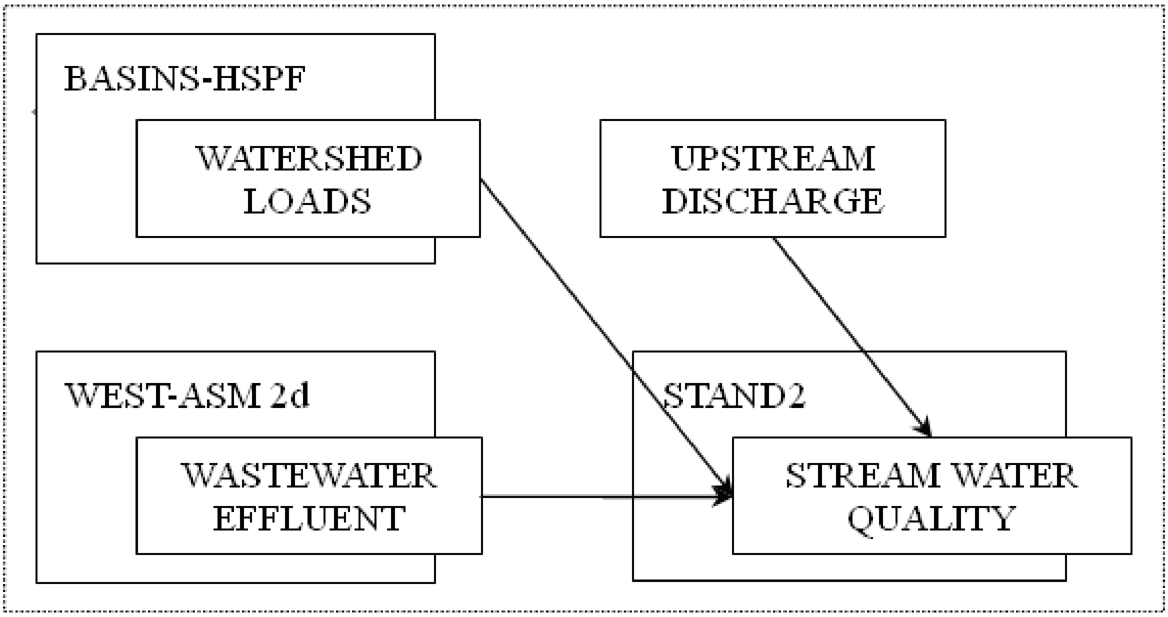


Figure 5-5: Components in watershed simulation system

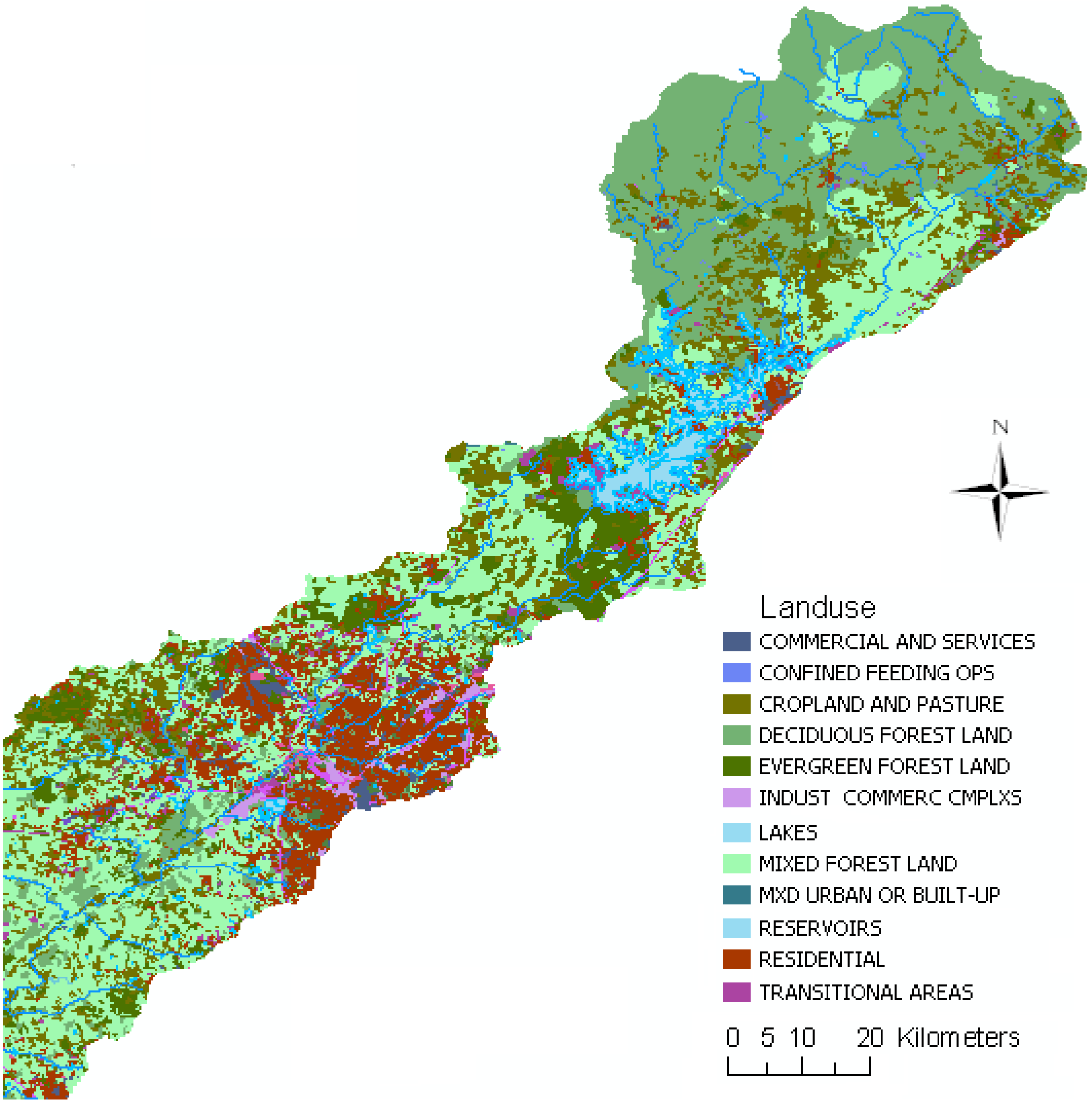


Figure 5-6: Watershed land use type

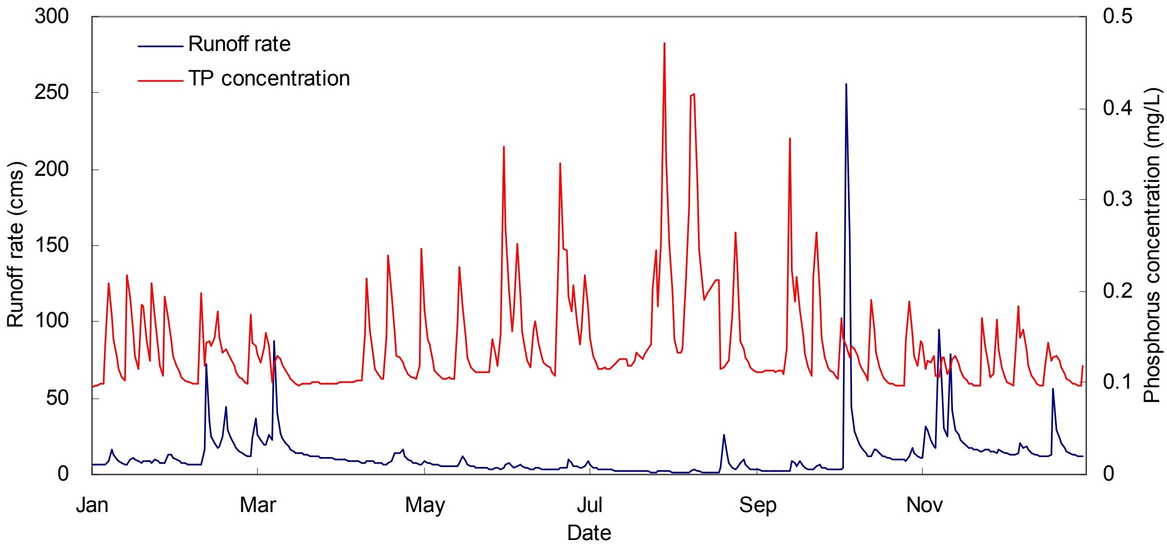


Figure 5-7: An example of nonpoint source load evaluation

(Sweetwater Creek watershed, 1995)

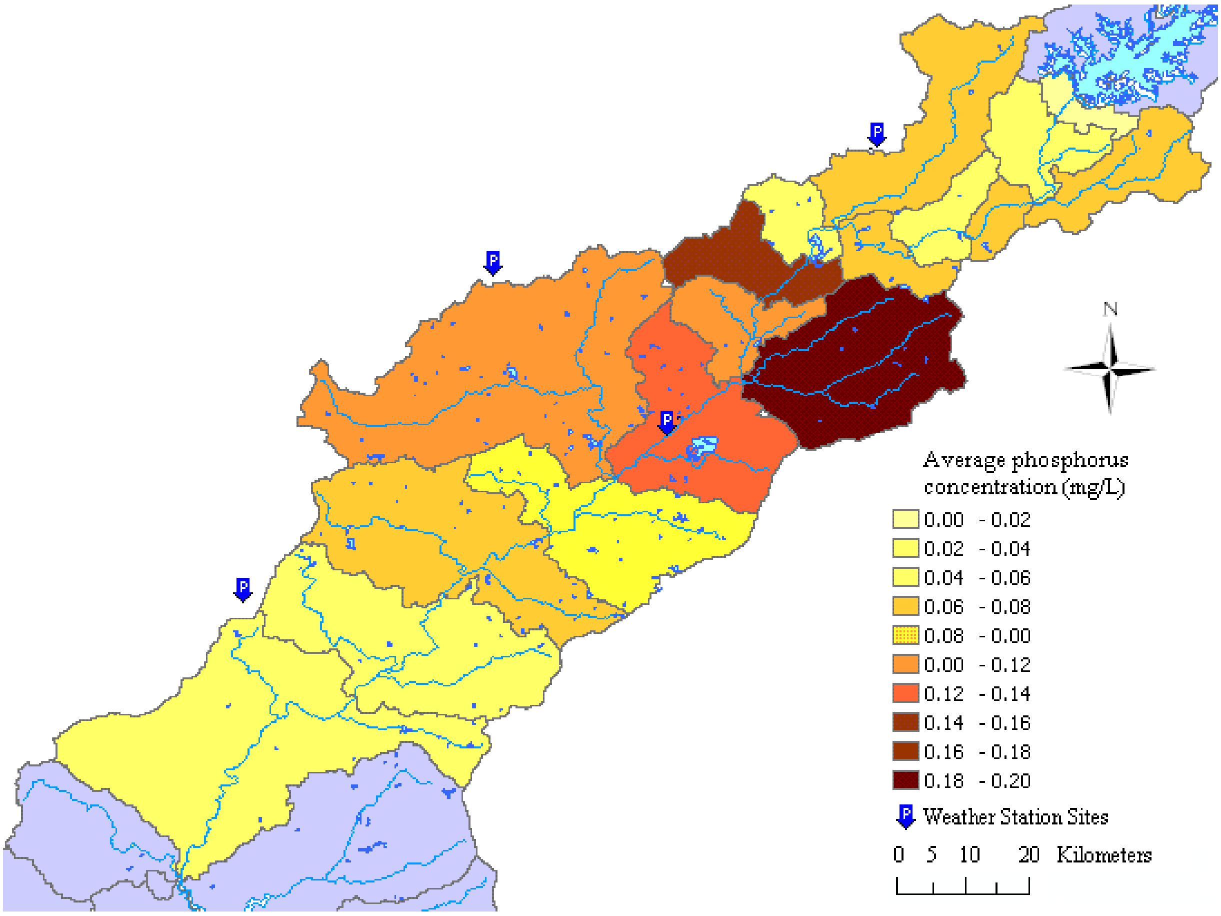


Figure 5-8: NPS distribution for each sub-watershed

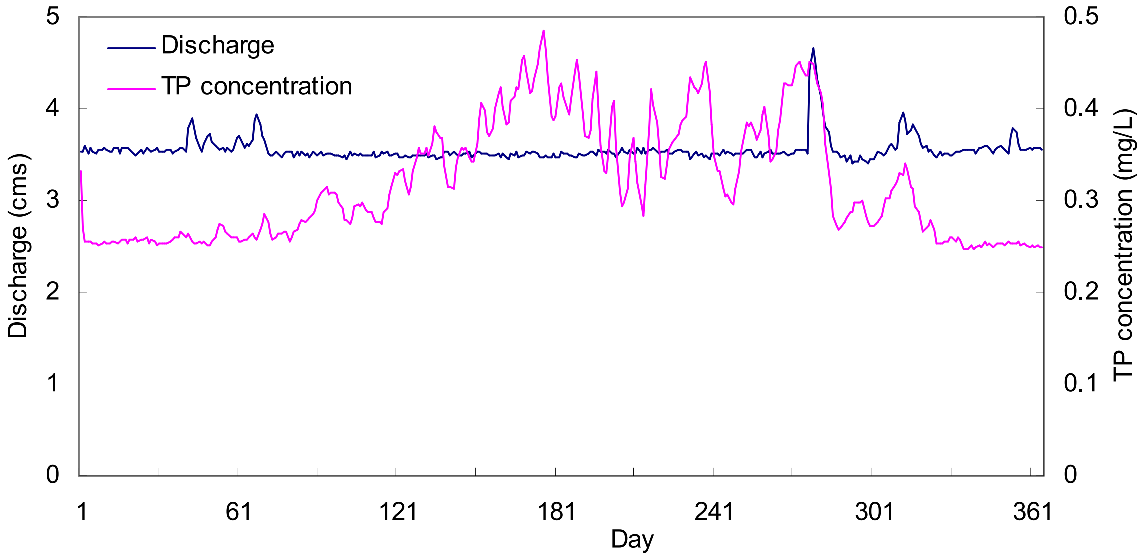


Figure 5-9: Discharge rate and TP concentrations

(R.M. Clayton WWTP, 1995)

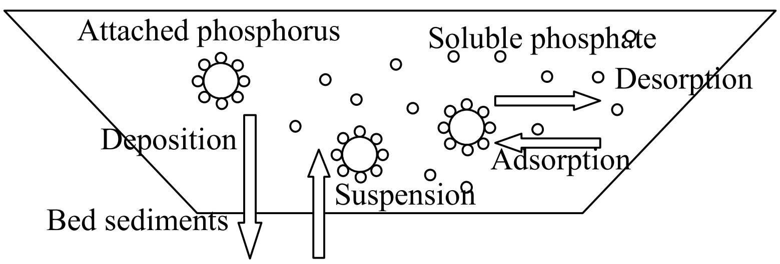


Figure 5-10: Sediment and phosphorus behavior in water column

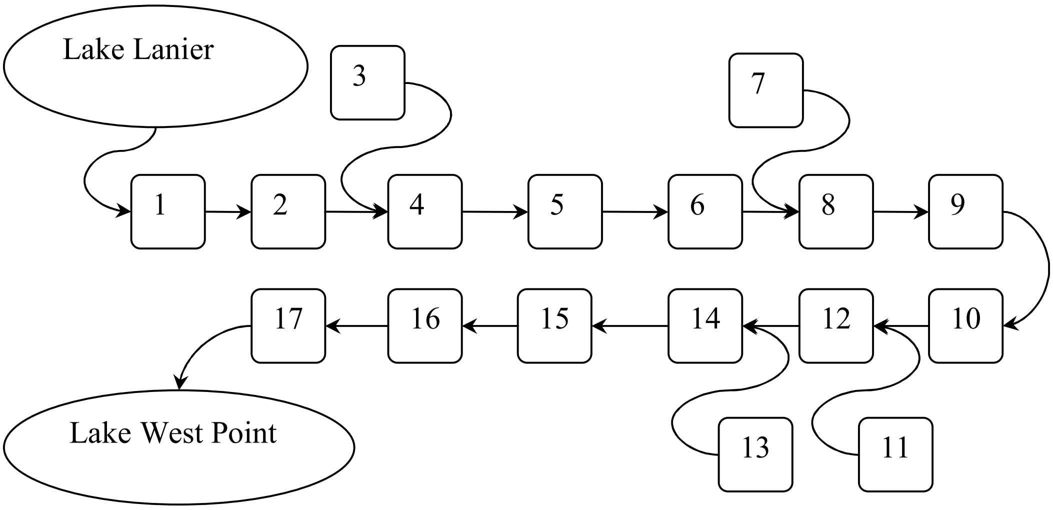


Figure 5-11: Schematic figure of river segments

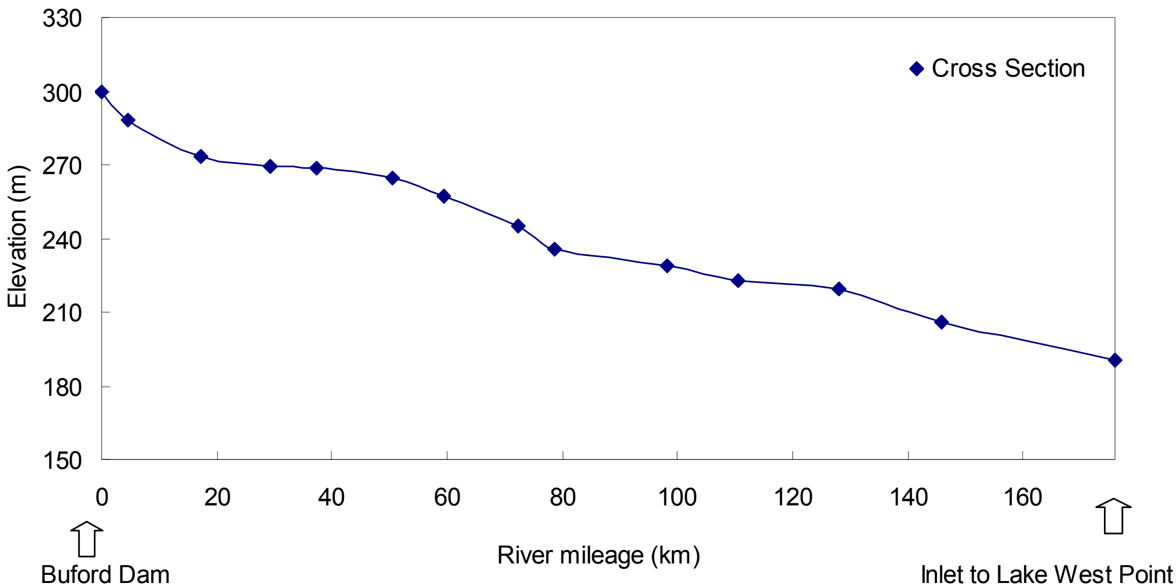


Figure 5-12: Elevation profile along the river

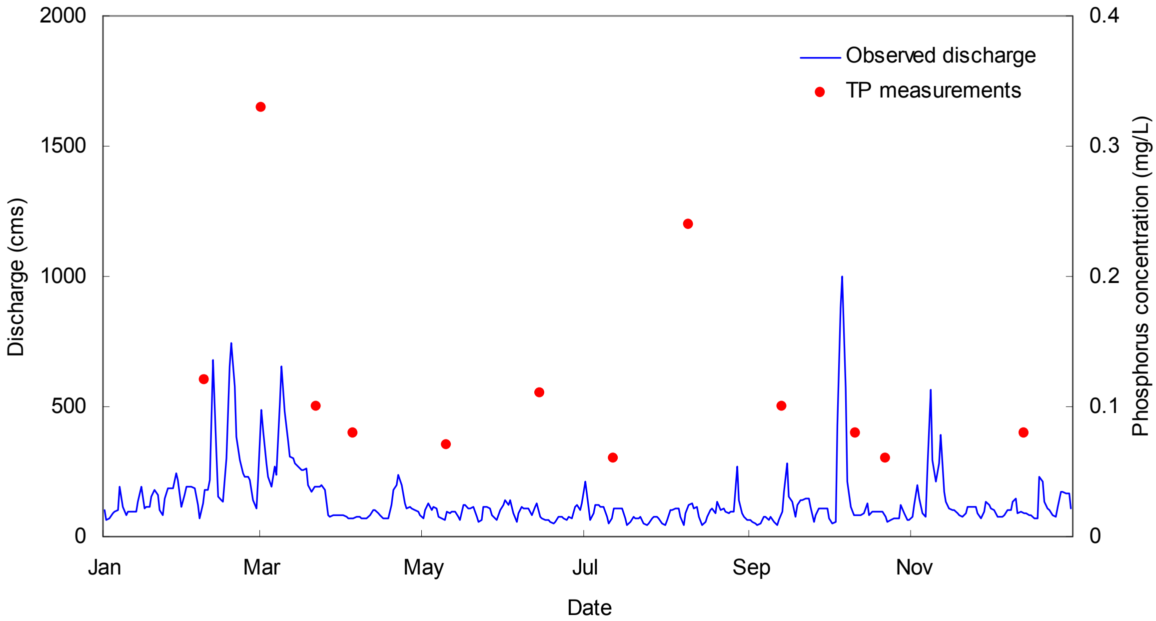
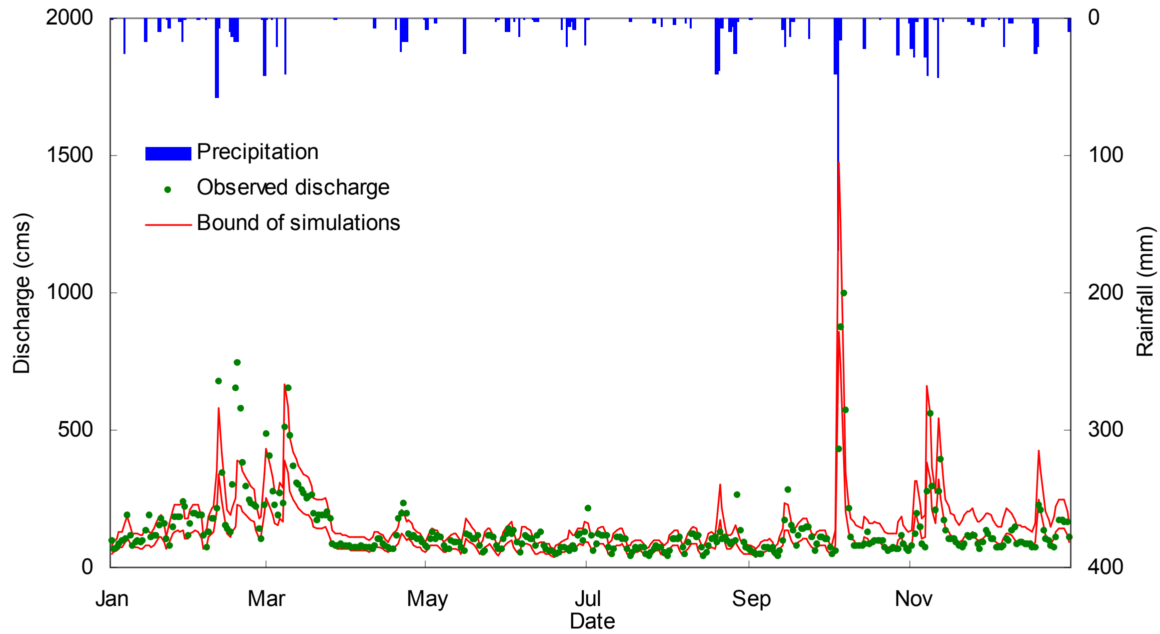


Figure 5-13: Monitoring data series

(At inlet of Lake West Point, USGS station 03328550, Franklin, Georgia 1995)



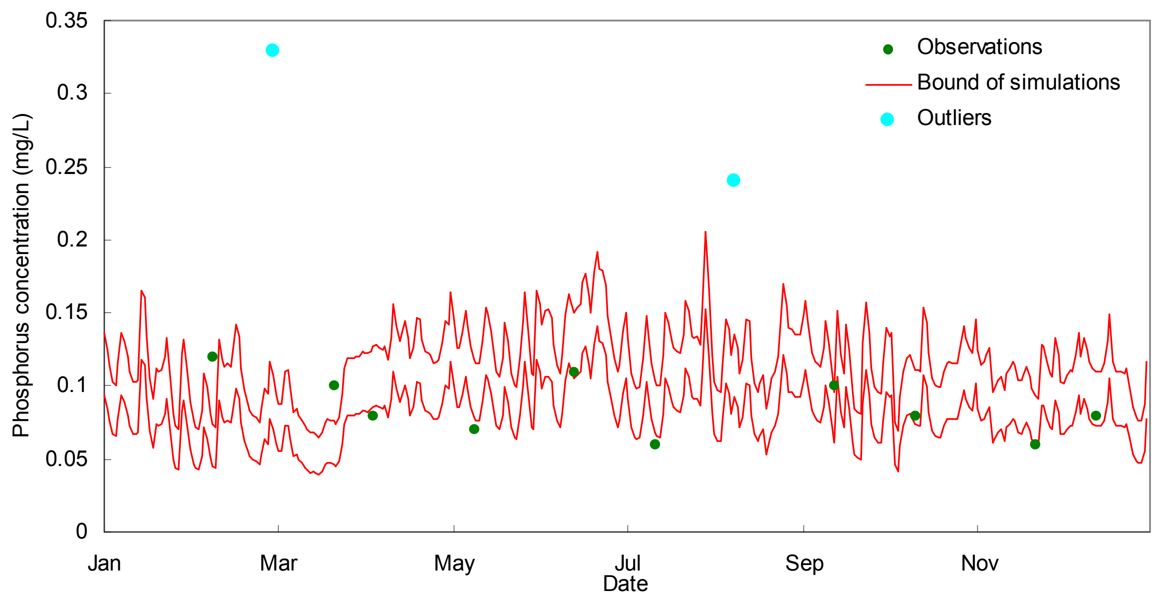


Figure 5-14: Simulation results under uncertainty

(At inlet of Lake West Point, 1995)

Chapter 6

A COMPUTATIONAL FRAMEWORK FOR TMDL MODELING

6.1 A framework for modeling under uncertainty

Environmental management and policies must be based on adequate and scientific understanding of the watershed and pollutant behavior, which ought to be achieved through a combination of modeling and the analysis of uncertainty. Uncertainty, and its influence in the identification and application of models, needs to be properly explored to ensure the quality of the model application and management-oriented tasks.

From this chapter, the Integrated Modeling under Uncertainty for Supporting Environmental Management (IMUSEM) system is assembled and applied for two example cases. It is constructed mainly by embedding the watershed model within a sampling-based uncertainty processing framework. It is essentially a framework of management-oriented environmental modeling, with particular consideration of the presence of substantial sources of uncertainty.

We begin by clarifying the uncertainty sources and evaluating their impacts on water quality conditions and pollutant loads. Again, uncertainty from each source is expressed as a probabilistic distributions for each parameter. Random samples are taken from these parametric distributions and substituted into the model system, for generating the trajectory of model outcomes. The distributions of these simulations of watershed pollutant yield and water quality reflect the impacts of assocaited uncertainties. The watershed model constructed in Chapter 5 will also be employed in this chapter. Herein Monte Carlo simulation is employed for analyzing the consequences of significant sources of uncertainties, in respect of illustrating their propagation through the assembled watershed modeling system, which is shown in Figure 6-1. We use the general framework and this specific case study to show how these various uncertainties can be properly evaluated on a consistent basis. This in turn will be informative in developing effective and reliable environmental policies, including those to be implemented via the mechanisms of the TMDL and water quality trading.

6.2 Evaluating the uncertain factors

Our understanding, and therefore our models, of watershed hydrological processes and their associated fluxes and transformations of the variables characterizing water quality are subject to significant uncertainties. This is especially so in respect of water quality and its transient behavior in response to precipitation events, not only in association with nonpoint-source discharges, but also point-source systems. Preliminary studies indicate that four major sources of uncertainty are affecting sediment and nutrient behavior in the Chattahoochee River as it passes through the Atlanta area (Osidele et al. 2003): (i) reservoir operations at the upstream Buford Dam, which determine the discharge pattern from Lake Lanier and consequently the stream flow at Atlanta; (ii) watershed loading resulting from precipitation-induced soil erosion, overland pollutant release and transportation; (iii) urban wastewater effluent as well as the effects of wastewater treatment plant operations; and (iv) in-stream processes of entrainment, deposition, phosphate adsorption and desorption. A key task here is to account for these uncertainties quantitatively and to assess the water quality conditions under the effects of uncertainty.

The nonpoint-source watershed loadings are usually believed to bear most significant uncertainties. These are greatly driven by transient precipitation events, hardly-measured diffused overland runoff and associated pollutant release processes. Within this context of uncertainty, 36 annual sequences of daily rainfall (generated from 1970-1995 historical data), are parameterized as an index of hydrological pattern (N_C) to describe climate variation scenarios. For the point-source loadings and their uncertainties, and given the techniques used for wastewater treatment, the effluent total phosphorus concentration is parameterized as (N_W), whose variation is between the current typical concentration of 0.3 mg/L up to the imposed limit, i.e., regulated by EPD's standard of 0.65 mg/L.

The system's upper boundary condition, water releases from Buford Dam, varies greatly from year to year. The category (i) of the above four sources of uncertainty is expressed bydifferent annual patterns of daily reservoir discharges, selected from the historic data published by the U.S. Army Corps of Engineers for the same 36 years. Its variation accords with the value of the hydrological year pattern index (N_C). A summary of variations in dam discharges is plotted in Figure 6-2. The average phosphorus concentration discharged from Lake Lanier is parameterized through an index (N_Q), ranging from 0.01 to 0.02 mg/L according to USGS measurements.

Upstream reservoir operations, nonpoint pollutant loads and urban sewage discharges constitute other external forcing functions, while the in-stream nutrient routing and transformation describe the internal processes of the river. The in-stream processes are characterized by a set of parameters associated with the attributes of the channel segments. These parameters reflecting fluvial processes are considered still to bear residual uncertainty, even though after the calibration conducted in Chapter 5. They are parameterized by an index (N_F), where N_F reflects all those candidate parameter vectors judged to have generated acceptable behavior during prior calibration. Therefore by this means, we are able to show the propagation of uncertainty from the model calibration process to the subsequent TMDL modeling task.

6.3 Simulating water quality under uncertainty

The simulation model, thus set up to mimic closely the context of metropolitan Atlanta in the Chattahoochee watershed, is the technical basis for exploring the influence of these uncertainties. The significant uncertainties are represented by random sampling in the Monte Carle Simulation framework. 1000 random points are taken from the joint probabilistic distributions of the parameterizations of the formerly above-mentioned four uncertainty categories. Then the model system is executed repeatedly with each sampling set. The datasets of generated model outputs are used as a basis for subsequent statistical analysis.

Estimated pollutant concentrations and loading amounts are expressed in terms of probability distributions, reflecting the consequences of uncertainty propagation through the model system. Once again, taking the inlet to Lake West Point as our reference spatial (output) location from the overall model, the cumulative probability functions of the model outputs, resulting from the propagation of uncertainties from all four of the above sources (in concert) - are shown in Figures 6-3, 6-4 and 6-5.

The evaluated constituents include the annual nutrient load amount, and the average and peak total phosphorus concentrations in the steam. Figures 6-3, 6-4 and 6-5 demonstrate the current water quality condition when accounting for uncertainty. We know watershed assessment is often based on the percentile attainment of water quality standards. Recalling the EPA's general standard we have summarized in the former section, i.e., stream total phosphorus concentration should not exceed 0.1 mg/L, we see that the current water quality condition meets the requirement at a percentage of 83% (shown in Figure 6-3). However, if we consider this stricter standard of 0.05 mg/L, we see it is generally never reached. Regarding the limit of phosphorus loading imposed by the Georgia EPD's watershed management plan (635 tonnes per year for Lake West Point, and this addressed watershed segment contributes 95% of the total nutrient influx to the lake), the evaluated annual loading amount, ranging from 250 to 530 tonnes (Figure 6-5), are completely compliant with it.

So far, with this integrated modeling-under-uncertainty framework and its successful application in the Chattahoochee watershed, we have constructed a computational tool for watershed study. This framework provides a substantial platform on which we can evaluate the strategies of water quality management, and enhance the robustness of the decision making process. The following section of this chapter will make a further illustration for TMDL development.

6.4 Evaluating the TMDL

6.4.1 TMDL in Chattahoochee Basin

We have described above on the construction of an integrated modeling system, in which a comprehensive watershed simulation model is coupled to a sampling-based scheme for uncertainty and sensitivity analyses. Here, we address now the topic of environmental management and illustrate the application of our computational framework for TMDL development. As summarized in the Chapter 2, the TMDL describes the maximum amount of pollutant that can be assimilated by the waterbody without impairing the capacity to meet the designated use. The TMDL is a widely used tool for preserving the water body. Here the modeling system is behaving as a linkage between an instream water quality target and pollution sources. The computation in previous sections has generated a rather clear nutrient budget for the Chattahoochee watershed, as well as evaluations of the associated uncertainties, which has provided a quantitative basis for now the TMDL development.

As an important strategy for achieving requirements of integrated watershed management plans, TMDLs have been conducted in a number of Georgia's major river basins. By the end of 2002, over 850 TMDL's had been approved in Georgia. Most of the them have focused on fecal coliform bacteria (pathogens), metals, sediments, and dissolved oxygen (DO) (EPA 2000c). Currently there are no TMDL plans for phosphorus in Chattahoochee watershed (there are programs for sediment and bacteria), but there is significant research concerning chlorophyll-A, for which TMDLs for lakes are currently being developed, and this is closely related with nutrients, such as phosphorus.

Here we should note that the TMDL is expressed nominally as a daily load, when actually it is discussed more frequently on an annual basis. Further, the following study is focused on the average of the annual series, even though the model system is working generally with a daily time-step.

6.4.2 Water quality standard

Standard setting is the first task of water quality-based management programs such as the TMDL. The applicable water quality standard is usually the numeric interpretation by EPA of their narrative water quality standard, linked to the designated uses for the water body of interest. Since the nutrient of phosphorus does not have an acute effect like pathogens, the State of Georgia Regulations do not include a numeric criterion, i.e. a specific standard for the concentration limit in the stream and river. Based on EPA's general recommendations, therefore, as mentionedearlier in this chapter, the total phosphorus concentration of 0.1 mg/L is selected as the applicable water quality standard here.

We do not choose the more strict standard of 0.05 mg/L, even if it is even more suitable for this case (at a point where river directly enters a lake or reservoir) because it is too far away from the currently known natural reality. It does not make much sense to discuss such a strict standard under present situations. Recalling that the Georgia EPD has a phosphorus load limit to Lake West Point, which is 635 tonne/year, resulting in an allowable average concentration of 0.147 mg/L, this seems to be too lax to ensure the health of Lake West Point, especially when considering the severe drought of recent years. Lake water volume has been shown to be decreasing significantly during the past three years. If we keep to the current loose limit, the lake will bear the risk of starting to trigger an irreversible process of ecological degradation. The standard of 0.1 mg/L is determined as a kind of compromise, therefore, and will serve the purpose of illustration.

6.4.3 Prior uncertainty and sensitivity evaluation

Since the prior investigation has revealed that the uncertain factors are highly affecting watershed pollutant behavior, a question for TMDL planning is: what are the relative significance of these factors and how can they be manipulated to ensure the attainment of the proposed environmental targets? Therefore, the prior evaluation of the uncertainty is conducted by the method of RSA.

Here the objective of RSA is to rank the importance of the uncertain constituent factors of the composite model, conditioned on the set of prescribed target model outputs (compliance with the standard). In this manner the relationship between the uncertainty sources and their contribution to the resulting attainment of the water quality target, which is an important attribute of the real system, is revealed. Furthermore, the evaluations of the sensitivity of each uncertain parameter serve to indicate the significance of their corresponding forcing functions and processes in the watershed system. The results are expected to facilitate the prioritization of adaptive TMDL implementation by focusing control actions on the identified key factors.

Specifically, for both the average and peak phosphorus concentrations, prescribing targets for water quality assessment are assumed as: 1) the average total phosphorus concentration should not exceed 0.1 mg/L; and 2) the peak total phosphorus concentration should not exceed 0.15 mg/L. For the RSA, these targets are used to distinguish between the behavioral and nonbehavioral realizations.

The major sources of associated uncertainty have been specified in the last section. Adopting the constructed comprehensive modeling with uncertainty assessment system, as well as the representative prior probabilistic distribution that accounts for significant uncertainties, Monte Carlo simulation is performed for generating the distribution of model results, instream nutrient concentration and loading amounts. Model outputs and corresponding values of parameters are classified into two sets, of exhibiting either behavior or nonbehavior, depending on whether or not they fall within the predefined constraints. This is followed by a K-S two-sample test performed on each input factor to assess the statistical difference between the parametric values of the two sets.

In the computation, 1000 random points are sampled on the parametric domain, in association with the defined numerical water quality target, of which 535/1000 are classified as behavioral simulations. This procedure is designed for simulating the propagation of these uncertainties through the modeling process, and more specifically, for enabling a "regionalized" analysis of sensitivity to reveal the significance of each uncertainty source on determining the attainment of the environmental target. The calculated K-S statistic is listed in Table 6-1.

We see from Table 6-1 that four factors are classified into Class A, being thus highly significance, while one is classified as Class B, of medium significance. The reason for this could be that the total phosphorus is somewhat conservative in its behavior in stream and rivers. The point source effluent limit N_W has the second highest significance, being only less than the influence of the variation in hydrological patterns which incorporate the precipitation and the upstream reservoir discharge pattern.

The analysis has revealed important attributes of the watershed-river system which could provide beneficial insights for TMDL planning. It suggests that watershed characteristics and external impacts are key determinants for pollutant behavior. We have noticed that natural external functions, such as climate factors, account for a larger part of the instream water quality variation in the Chattahoochee River. However, since this is beyond management practice, in which we are more interested for TMDL implementation, the other factors will be discussed here. We will concentrate on these factors which determine the watershed pollutant loading and wastewater discharge.

6.4.4 Evaluating WLA and LA

The TMDL allocates the total allowable pollutant load to waste load allocations (WLAs) for point sources and to load allocations (LAs) for other nonpoint sources. The WLAs and LAs in the TMDL provide a limit on the amount of pollutant sources in order to prevent the waterbody from exceeding the applicable water quality standard. To evaluate the TMDL for this segment of the Chattahoochee River, we continue with on the numeric interpretation of the water quality target, which is that the instream total phosphorus concentration should not exceed 0.1 mg/L at the inlet to the downstream reservoir. The simulation under uncertainty conducted in the previous chapter (Figure 6-3) has shown that under uncertainty water quality can meet the target standard at a probability of 83%. The purpose of TMDL plan is to control the pollutant discharge with a maximum load limit in order to achieve complete compliance with the water quality standard.

We choose the point source effluent limit N_W as the operational parameter for achieving the target of the TMDL based on the following: 1) point sources are important and account for a large portion of the total pollution load in this watershed; 2) the point-source discharge limit significantly determines the variation of instream pollutant concentration according to the prior uncertainty and sensitivity analyses; 3) it is measurable and possible (and easy) to be manipulated in practice, compared with nonpoint sources, which we can not regulate at present; and 4) the control of point sources can be realized though various optional tools, such as through the mechanism of water quality trading.

Since point sources in this area are regulated by the NPDES (refer to Table 6-2), what we need for the TMDL is to improve and enforce it through the WLA. If the concentration limit for total phosphorus in the effluents of the point sources is assigned as 0.35 mg/L, then the resulting instream water quality will basically meet the water quality standard, with the uncertainty included in the evaluation. Figure 6-6 shows the distribution of average phosphorus concentration, which exhibits a to-left shift from Figure 6-3. The computation results show that with such a wastewater effluent limit for phosphorus, we have a 99% confidence in the assurance of instream water quality. This evaluation result will be the basis for the TMDL development.

Our choice on the limit of 0.35 mg/L for wastewater effluent is not an arbitrary decision. It is based on a comprehensive uncertainty evaluation and screening process. With different scenarios for the wastewater effluent standard, when the phosphorus concentration limit is set within the range of 0.3 to 0.75 mg/L, we have examined the response of instream water quality to such variation in this operational parameter. We see in Figure 6-7 that with the limit of 0.35 mg/L, the range of possible instream phosphorus concentrations (between percentiles of 1% and 99%) will be 0.054 to 0.1 mg/L. This is compliant with the water quality standard.

Based on this computational analysis, the TMDL scheme can be generated. The WLA (point sources load limit) and LA (nonpoint sources load limit) are evaluated and listed in Table 6-2. If we compare this TMDL scheme with the Lake West Point phosphorus limit in EPD's watershed management plan, where a limit of 635 tonnes is suggested, the loading permit generated by this study is much more conservative.

What is more, WLA is easily allocated to the point source dischargers within the context of the NPDES, but for LA the allocation for nonpoint sources is a little bit more complex. Fortunately, the spatial distribution of nonpoint sources in each subbasin throughout the watershed has been evaluated by the model of HSPF. We find that the allocation strongly depends on the watershed simulation result, which means, since there is not discharge permit enacted for regulating nonpoint sources, the allocation of LA throughout the watershed can be set as their current level of pollutant load, as listed in Table 6-3.

Taking the hydrological year of 1995 as an example, with the scenario that the TMDL plan suggested above is implemented, the resultant daily time series of total phosphorus concentration and load at the inlet of Lake West Point is shown in Figures 6-8 and 6-9. These two figures are generated by the computations for which every parameter value are set as same value except N_W are different with 0.65 (for without TMDL scenario) and 0.35 (after implementing the TMDL suggested above). Compared with the current simulated daily water quality variations in the absence of the TMDL, for which the under-uncertainty version is displayed in Figure 5-14, we can see an obvious abatement of daily total phosphorus concentration resulting from the TMDL application. It shows us that this TMDL allocation will provide substantial water quality benefits, as expected, despite various types of uncertainty potentially undermining the analysis. In Figure 6-9 we also notice that the water quality improvement resulting from the TMDL is more significant during low-flow than high-flow conditions. This is consistent with the focus of this TMDL on limiting discharges from point sources, which are normally more significant during dry periods.

6.4.5 Determining Margin of Safety

The margin of safety (MOS) is part of the TMDL development process. There are two basic methods to determine the MOS: implicitly incorporate the MOS using conservative assumptions for modeling when developing TMDL allocations, or explicitly specify a portion of the total TMDL as the MOS and use the remainder for allocations to dischargers (EPA 2008b). It has been recommended that EPA should abandon the current practice of arbitrarily assigning the MOS in favor of an explicit analysis of uncertainty (NRC 2001). In our research, therefore, we use the implicit method by incorporated it implicitly into the uncertainty analysis process, generating the TMDL by ensuring the computed water quality, in spite of the uncertainty, is not beyond the standard.

Considering the critical situation, when the instream phosphorus concentration is just as high as the standard (0.1 mg/L), the calculated annual load (in combination with the annual total discharge amount) to the downstream reservoir is 473 tonnes. Then the MOS is 143 tonnes per year, which is 30.2% of the total TMDL. By another method, if we exclusively depend on our simulation results including consideration of uncertainty, the evaluated upper bound for the TMDL is 455 tonnes per year, so that the MOS will be 125 tonnes per year, i.e. 27.5 % of the TMDL.

6.5 Summary

The TMDL is an ambient-based watershed management approach. In this simulation study, therefore, we start from the requirements of instream standards, using the models to calculate the allowable watershed pollutant load. The method we have employed in this study has shown significant promise for accounting for uncertainties in the TMDL development process. In this chapter, a methodology has been illustrated to comprehensively evaluate and process the involved uncertainties, but it has not covered all aspects thereof. For example, long-term population and economic growth and climate change will inevitably influence on the environmental conditions and produce new challenges for the TMDL plan. City growth may bring more pollutant loads into the waterbody and global warming will substantially increase the risk of aquatic ecological degradation by algal blooms. More significantly, the drought of the past several years has apparently altered the water resource conditions. The extra uncertainties caused by these predictable and unpredictable factors need to be further evaluated and incorporated into a scientific study. These potential risks may require us to assign a higher magnitude of MOS for possible scenarios and more stringent limits may have to be implemented for watershed management. Correspondingly, in our framework, it should be rather beneficial to incorporate and evaluate these long-term uncertainties.

Through this case study, we have illustrated an application paradigm of our framework of Integrated Modeling under Uncertainty for Supporting Environmental Management. Next, we will extend it into another multidisciplinary topic, water quality trading, to explore the uncertainty, modeling and environmental management problem within a more complex setting.

Table 6-1: Significance of uncertain factors

Symbol	Description	d	Z	Class
N_C	Index of annual hydrological pattern	0.429	6.7655	A
N_Q	Upstream reservoir discharge concentration	0.136	2.1404	A
N_W	Point source effluent limit	0.374	5.8965	A
N_F	Fluvial parameters	0.086	1.3595	B

Table 6-2: Evaluation of the TMDL allocation

Unit (tonne/year)	Average load	Lower bound	Upper bound
LA	190 (57.6%)	120	265
WLA	115 (34.8%)	90	140
Upstream load	25 (7.6%)	10	50
Sum	330 (100%)	220	455

Table 6-3: Nonpont source allocations for subbasins

Subbasin	Load (tonne/year)	Subbasin	Load (tonne/year)
No. 1	1.64	No. 10	6.49
No. 2	3.44	No. 11	20.40
No. 3	5.86	No. 12	16.93
No. 4	1.95	No. 13	29.99
No. 5	3.13	No. 14	14.22
No. 6	3.62	No. 15	18.37
No. 7	11.60	No. 16	17.57
No. 8	3.50	No. 17	24.97
No. 9	6.31		

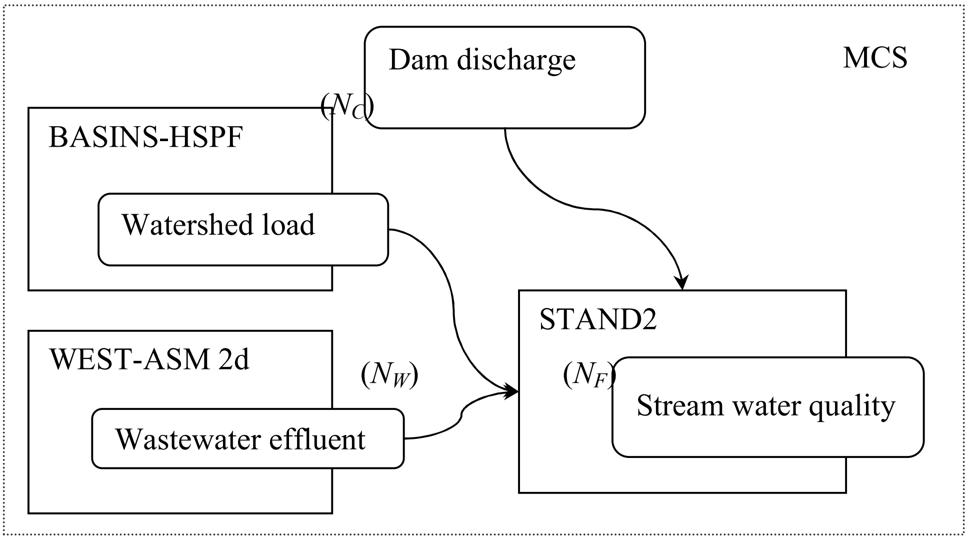


Figure 6-1: Integrated uncertainty evaluation system

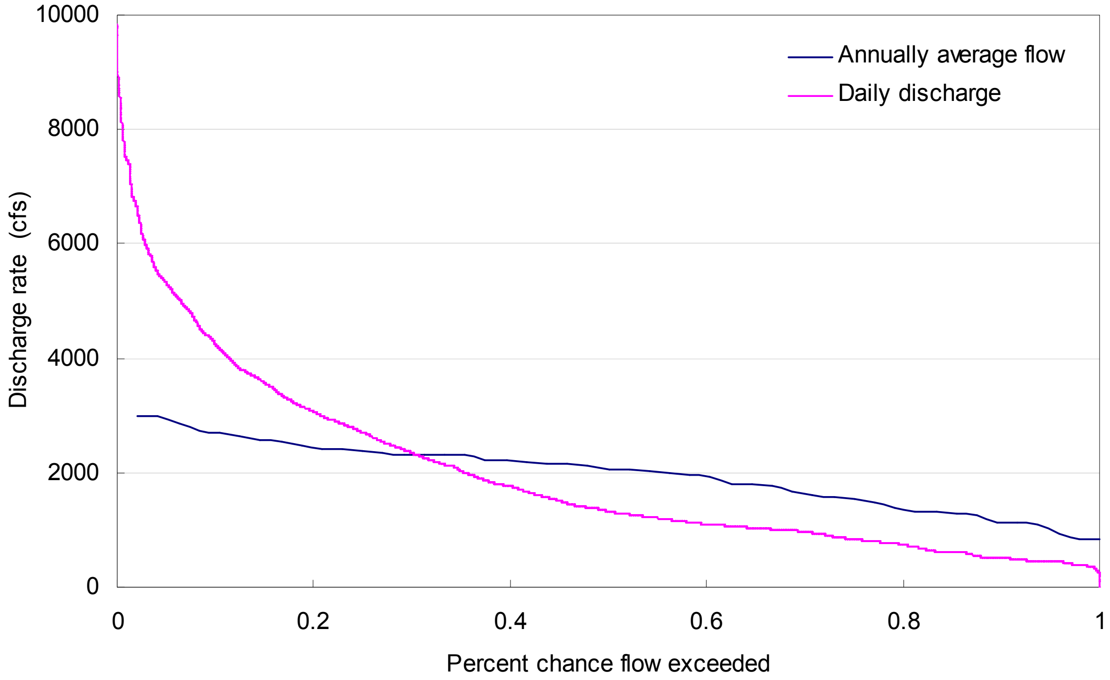


Figure 6-2: Flow-duration plot for Buford Dam discharge

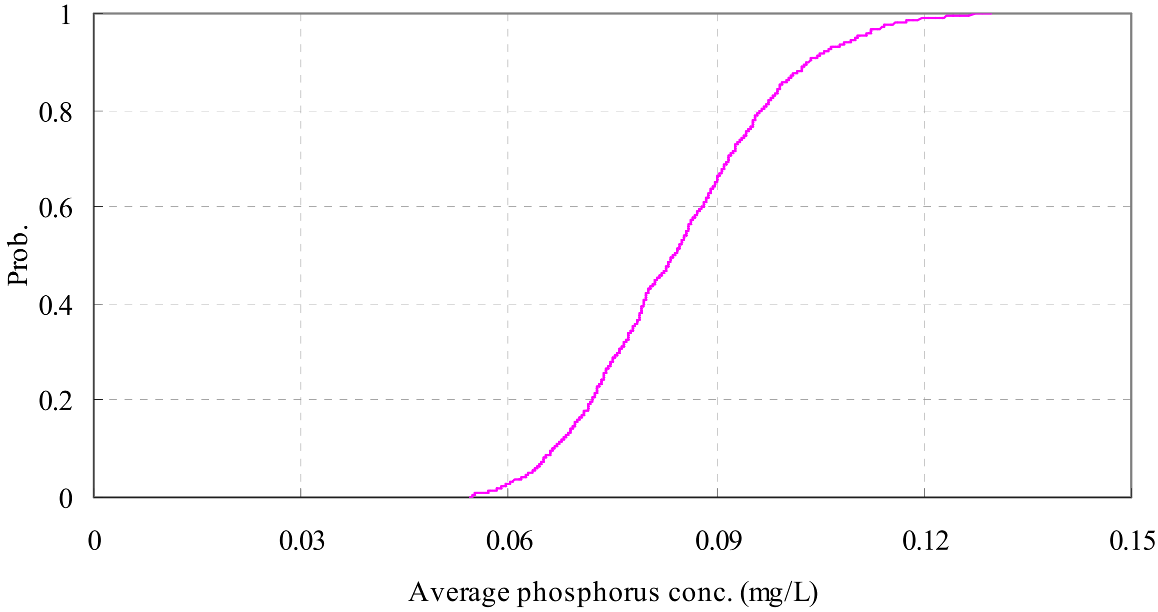


Figure 6-3: CDF of simulated average TP concentration

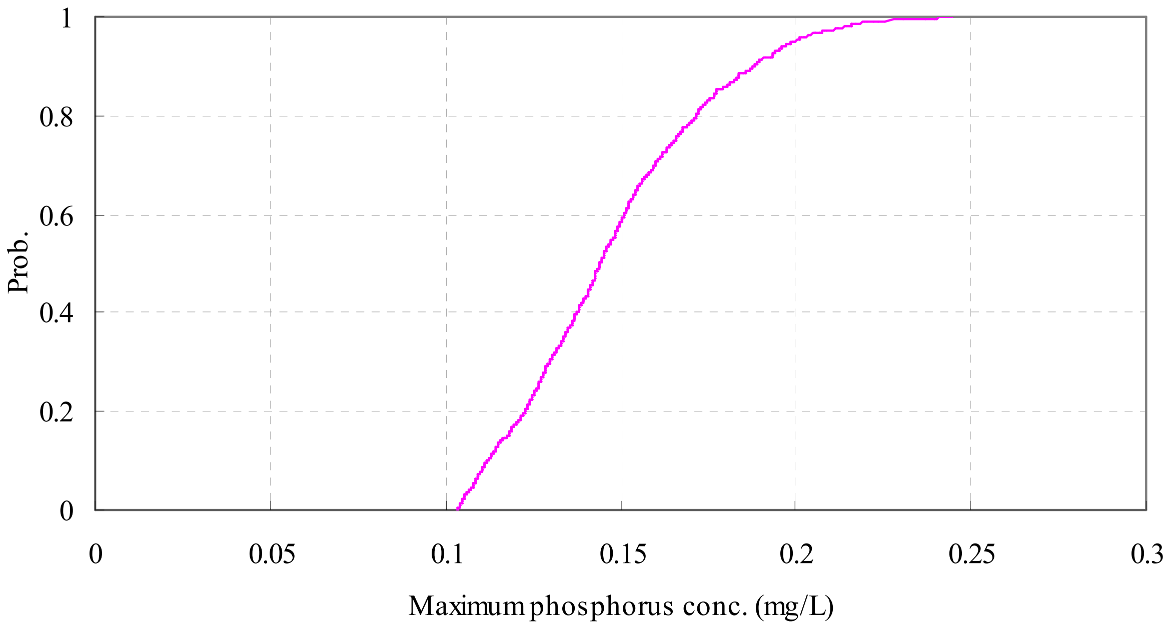


Figure 6-4: CDF of simulated peak TP concentration

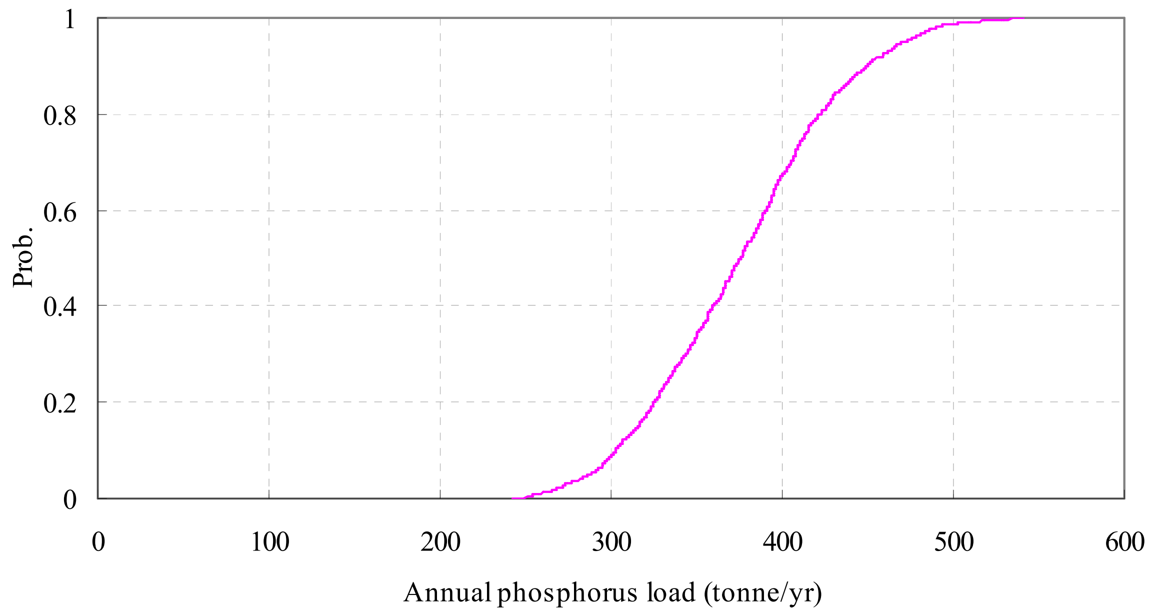


Figure 6-5: CDF of simulated annual phosphorus load

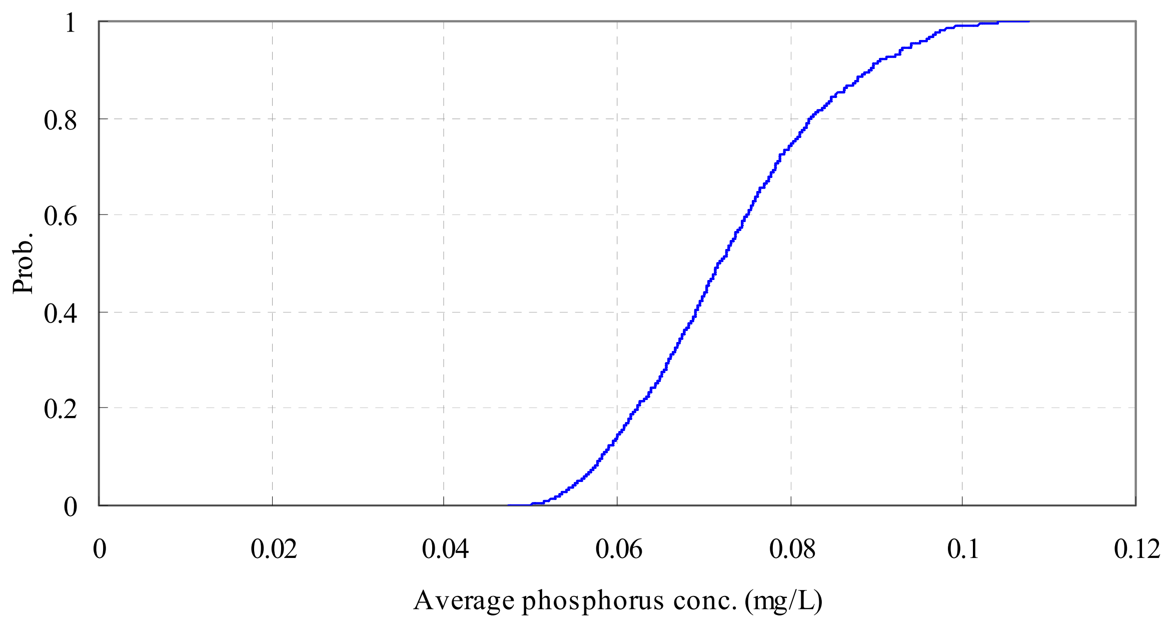


Figure 6-6: CDF of simulated average TP concentration

(Water quality target of TMDL implementation)

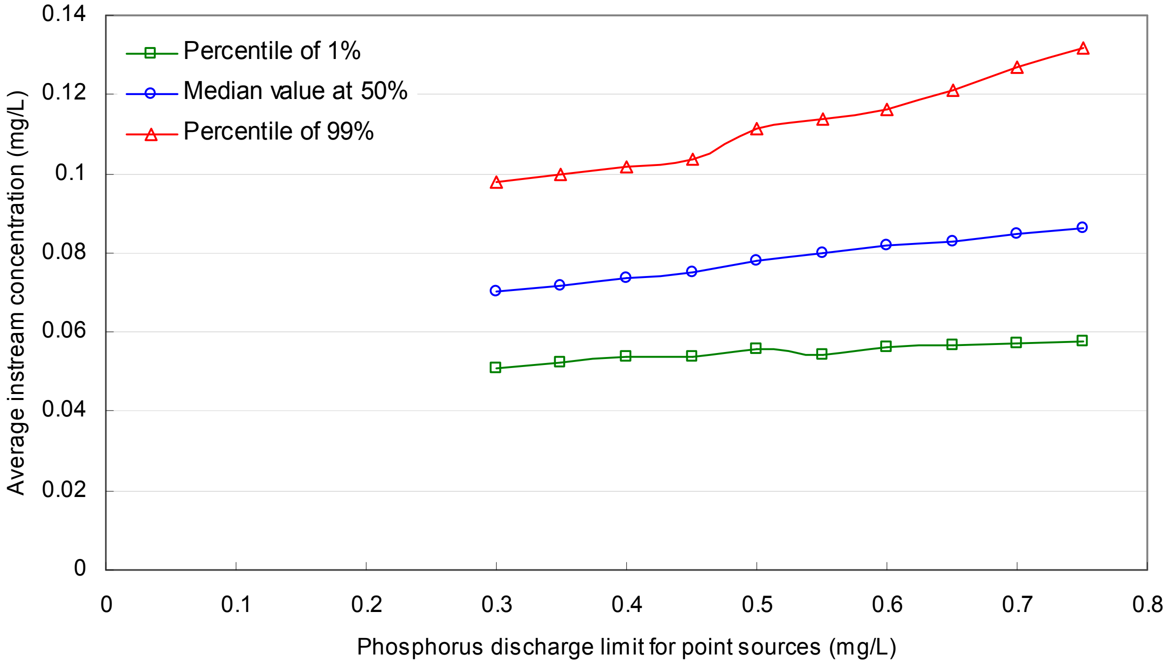


Figure 6-7: Response of phosphorus concentraion as a function of the wastewater effluent concentration limit

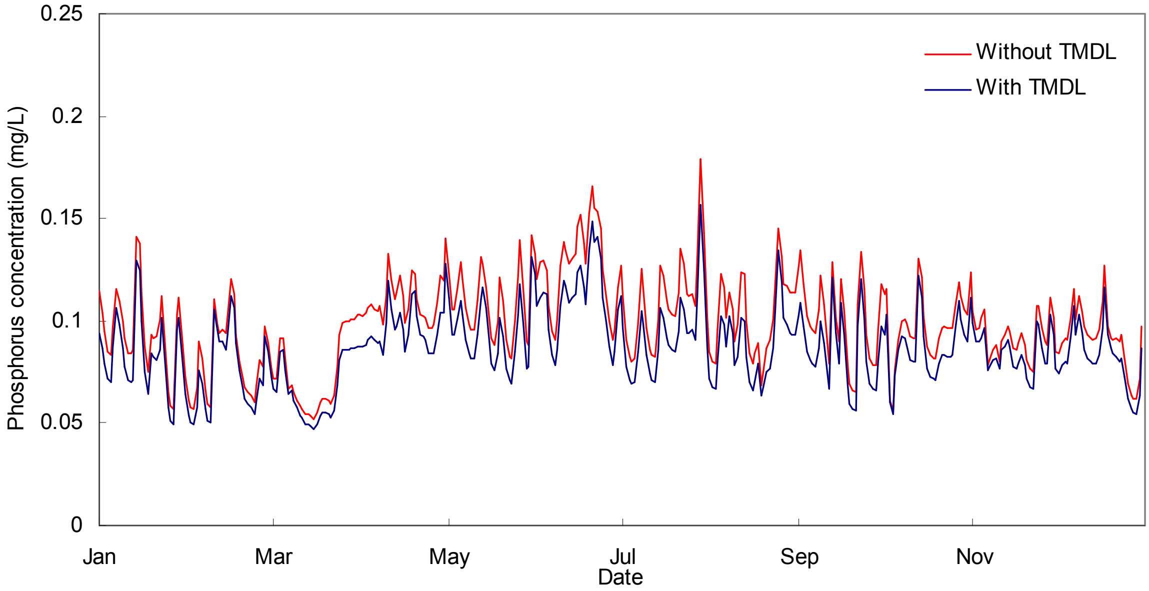


Figure 6-8: Effects of TMDL implementation on phosphorus concentration

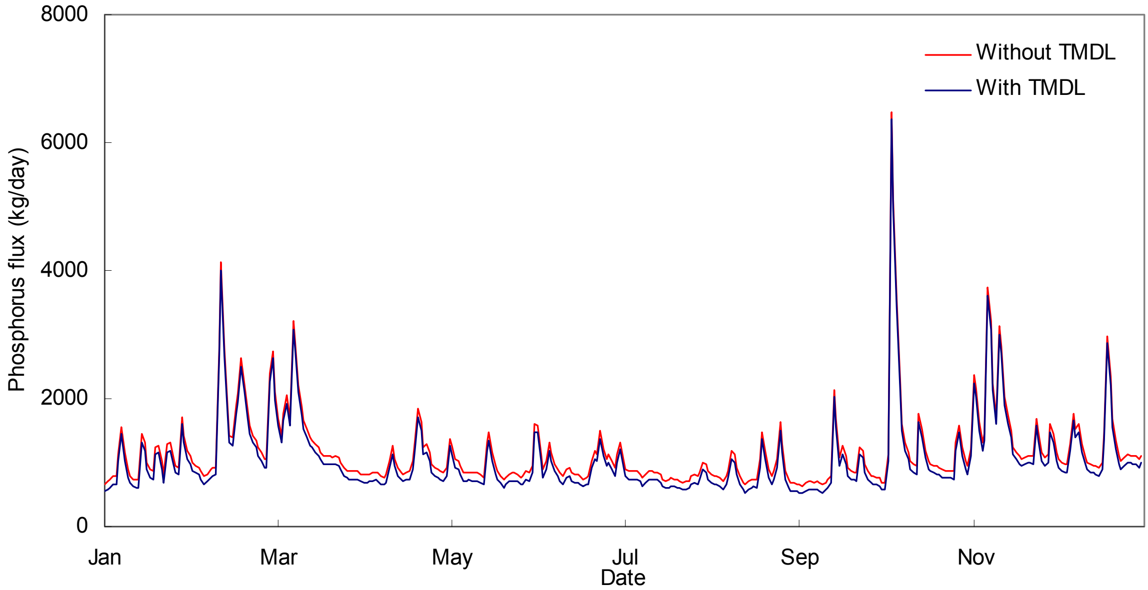


Figure 6-9: Effects of TMDL implementation on phosphorus flux

(At inlet of Lake West Point, 1995)

Chapter 7

EXPLORING WATER QUALITY TRADING UNDER UNCERTAINTY: A SIMULATION STUDY

7.1 Introduction

The previous chapter has illustrated a primary application of our integrated watershed study framework and shown how the various uncertainties in simulating of a natural watershed system can be evaluated on a consistent basis in order to generate a reliable TMDL plan. In this chapter, we will focus on another watershed management tool, water quality trading, to extend further the performance of this dissertation's modeling-uncertainty framework.

Water quality trading is a good example for discussing scientific environmental management. As stated in Chapter 2, it is an innovative and immature approach with multidisciplinary features - applying the market approach to the problem of pollution control and water quality management. Another important feature is that it involves a large amount of uncertainties. They are transferred, amplified and ultimately affect the performance of policy implementation. Therefore, a clear account of the consequences of such uncertainty must be evaluated before proposing trading plans, in order to ensure their operational effectiveness.

The key motivating questions to be answered by this chapter include the following:

(1) What are, and how do we evaluate, the uncertainties involved in water quality trading programs?

(2) Under these uncertainties, how would our computational research support watershed management through trading?

In earlier chapters, we have assembled a rather complete model for a watershed, wherein the dynamic behavior of point sources, together with that of nonpoint sources and stream routing processes, can be properly accounted for. The analysis in this chapter will continue to be tightly based on this same computational methodology. Furthermore, in order to explore water quality trading within a wider perspective, we will extend the coupled modeling and uncertainty analysis system with a component of economic analysis, for achieving a more integrated tool for substantially supporting watershed management.

Regarding the issue of water quality trading, a large mount of uncertainty comes from various sources, such as measurements, assumptions or structure of the computational method (models), development scenarios, and social-economic issues. Once more RSA computations are conducted for revealing the significance of each uncertain factor, conditioned upon the designated targets of water quality trading. These analyses might produce useful insights for the design of more reliable trading programs.

In brief, a new pollutant-trading-under-uncertainty research framework is composed in this chapter. In addition, this kind of consistent "*in silico*" evaluation is especially important at a time when there is a strong aspiration to see pollutant trading schemes implemented, but little direct evidence of their successes/failures in actual practice.

7.2 Feasibility in the Chattahoochee watershed

At present, like most Georgia watersheds, Chattahoochee river phosphorus is unregulated, or regulated at a level insufficient to support water quality trading. Thus the study of water quality trading is at the stage of a preliminary feasibility investigation. It is generally considered that water quality trading projects will be more effective under circumstances with 1) significant point sources and nonpoint sources in a watershed with comparable amounts of the two types of discharge, 2) motivations to facilitate pollution reductions such as a TMDL, 3) sources facing different costs to control the pollutant of concern, 4) willingness of watershed stakeholders and the state regulatory agency to participate, and 5) a good pollutant monitoring system (Ng and Eheart 2005).

According to these requirements, earlier investigation of Georgia watersheds has indicated that the Chattahoochee watershed is one of the more suitable watersheds for the application of trading programs. It has several characteristics that favor the feasibility of water quality trading, including environmental suitability, regulatory incentives, availability of participants, economic incentives, and stakeholder responsiveness (Rowles 2004).

These evaluations concluded that the opportunity for water quality trading in Georgia is somewhat limited by present regulatory conditions (Rowles 2005), principally due to the absence of an important prerequisite, a clear TMDL plan for nutrients, and the fact that non-point sources are not regulated (King and Kuch 2003). In the last chapter, we have generated a clear phosphorus budget for the watershed of interest, based on which a TMDL scheme has already been derived. This TMDL can be considered as a cap or baseline, or as a incentive for potential water quality trading programs, when the TMDL cannot not achieved and some dischargers need to make reductions while facing high costs.

The two lakes located upstream and downstream of our study area form a natural boundary for the potential water quality trading market. The downstream Lake West Point receives all the pollution discharged from this watershed and thus is our focus. Because lakes and reservoirs are much more sensitive than the streams and rivers to higher nutrient loads, and they are also normally where ecological impairment most probably happens, as in “hot spots”, the inlet to Lake West Point is crucial. It is there where the success or failure of trading will judged.

The TMDL evaluation of Chapter 6 suggests a limit of 115 tonnes per year for total point sources and 190 tonnes per year for nonpoint sources for this segment of the Chattahoochee River for compliance with water quality standards. However, for such a dynamic watershed system, various scenarios will possibly happen to disturb the phosphorus load allocation under this TMDL. For example, continuing population and economic growth in Atlanta area will bring more pollutant discharges into the river. The change of natural factors, such as the threat of climate change, may also require reducing the watershed pollution load. And if the water quality standards are changed to be more stringent, which is actually shown to be a trend of watershed management, the TMDL will decrease correspondingly, and then the reduced allocation of discharge permits will oblige the dischargers to achieve a higher pollution abatement. In fact, some of the wastewater plants have proposed to upgrade their phosphorus removal efficiencies to meet a tighter effluent limit of 0.13 mg/L or 0.3 mg/L (Rowles 2004). The requirement of further reductions by point sources provides the regulatory incentive for the adoption of water quality trading. This is in reality happening in the Chattahoochee watershed.

7.3 Dual targets and associated factors

The goal of water quality trading is notably consistent with two of the triple bottom lines of sustainability: environmental benignity and economic feasibility. Correspondingly, for evaluating the performance of water quality trading programs, we also have two criteria, which are water quality improvement and financial benefit.

Specifically, the target of water quality trading is to achieve benefit on the both issues of water quality and the economic account: after the transaction of water quality trading happens, the resulting water quality (or pollution load under a TMDL) should be no worse than the situation without trading and all the participant parties should gain financial benefit. If either of these criteria is not attained with confidence, we will conclude that the proposed program is ineffective or unsuccessful. In addition, these two criteria are also used for the behavioral definition within the RSA framework. In the following sections, we will make a rather comprehensive uncertainty analysis of the important factors included in water quality trading, then construct a system incorporating both environmental and economic components, feed these uncertainties into the system to evaluate their impacts, and assess their respective significance conditioned by the dual targets of this policy.

With respect to these two essential criteria, the methodology used here comprises two major parts for the environmental and economic perspectives: water quality evaluation and financial analysis. They interact with each other and act jointly to determine the potential effectiveness of water quality trading markets. For each perspective, a number of factors should be examined, since many of them are believed to be bear large uncertainties, which might impair the attainment of trading targets.

For the Chattahoochee is concerned, the important factors in the environmental dimension include not only those already evaluated in Chapter 6, but more significantly here, the magnitude of the trading market, which determines the volume of pollution to be transported. In the financial analysis component, the uncertainty sources are primarily identified as the cost estimates of pollution control. When we attempt to evaluate the nutrient removal cost for different dischargers, as well as the transaction cost for constructing and operating the trading market, there depend on many factors from various fausets of the social-economic community, and their variations are extremely large. In the following paragraphs, we will try to properly identify and quantitatively account for them.

7.4 Evaluating the environmental constituents

7.4.1 Pollution sources

As a typical market-based tool for water quality management, most water quality trading programs adopt the form of baseline-and-credit, under which a pollution source in a watershed could generated tradable credit only by achieving a certain amount of pollution abatement beyond the required reductions in specific pollutant loads. Then through the trading market, if another polluter who needs to discharge more than its initial assigned permit and has a higher cost to eliminate these additional pollutants, they can buy the credits.

In water quality trading programs which include both point and nonpoint sources, the nutrient discharge credits are usually traded from nonpoint sources to point sources. Among the watershed nonpoint source dischargers, agricultural sources are normally believed to have the potential for pollutant abatement with lower cost, so they are often considered as the major participants for water quality trading. In Chapter 5, we have already calculated the spatial distribution of nonpoint pollution sources throughout the whole area of interest. From the map of land use type, the agricultural areas are mainly identified to be distributed in the 7th, 13th, and 17th sub-basins. In this case, these farms are the potential sellers of nutrient discharge credits. This is not to say that other types of diffused pollutant sources, such as urban runoff, cannot participate in water quality trading projects, but only the agricultural sources are evaluated here in order to illustrate our framework.

With regard to the potential buyers in the water quality trading market, they are normally considered to be those point sources who need to make more pollution abatement beyond current capacities while facing a higher control cost. In Chapter 6 we have generated a TMDL plan for this watershed, for which a more stringent phosphorus concentration limit is imposed on point-source dischargers, and this could be a stimulant for the application of trading programs. In addition, population growth and urban development in Metro Atlanta area will definitely continue at a higher or lower speed in the future, and inevitably, elevated amounts of municipal wastewater will be discharged into the Chattahoochee River. However, since the current stream water quality and pollution load are already equal to or worse than the critical values to meet the requirements of the designated water usage, there are no more discharge permits to be issued. Thus, the wastewater treatment facilities have to expand their capacities or upgrade their processes to eliminate the extra pollution load and maintain the current limit, probably with a rather high cost. However, the method of water quality trading provides alternatives for the plant instead of neutralizing the pollutant all by itself. Under a WQT framework, these facilities have one more option, which is to purchase a discharge permit from the trading market. And the price of that pollution credit is very probably lower than the original cost for upgrading.

Alternatively, and just as realistic for the Chattahoochee watershed as adopting more stringent effluent limits, the discharge permit for many point-source discharges might shrink to a value below the current discharge rate. Plants would then need to make extra reductions and would accordingly consider participating in the trading market. Either scenario will result in the requirement of achieving more phosphorus reduction and this is the major incentive for the adoption of cost-effective pollution management tools like water quality trading. In the following computational assessment, we assume that a certain amount of phosphorus (E_L, which is estimated to be 5 to 10 tonnes per year, 5% to 10% of the total point source load) needs to be reduced by point source dischargers and seek a cost-effective means to do so.

7.4.2 Pollution reduction by BMPs

Best management practices are methods that have been determined to be the most effective and practical means of preventing or reducing pollution. These practices are often employed in agriculture, forestry, mining and construction. Under the baseline-and-credit form, when a portion of pollutant discharges are eliminated by means of control practices, such as implementation of a certain BMP strategy, a tradable credit will be generated and available for marketing. Much research and many projects have shown that a suitable BMP could substantially decrease the concentration of various pollutants including phosphorus (WERF 2008). With respect to the watershed addressed here, BMPs are enthusiastically proposed for farming management and controlling broiler litter. It is expected that the manure removal from the watershed and treatment will effectively reduce the nutrient release. However, compared with wastewater treatment process for point-source control, efforts to mitigate pollution with BMPs are still in the early stages of development. The amount of pollution abatement that can be achieved by a BMP, and its effectiveness, are rather uncertain.

The EPA, working with partners in industry and the academic community have established and published best management practices for agriculture and livestock yards, soil erosion, waste treatment, pesticide and fertilizer applications. More specific, evaluations of the effect of some widely used BMPs, mainly on nonpoint sources, are summarized and listed in Table 7-1 (Palace et al. 1998; WERF 2008). Recalling the fact that agricultural lands account for about a quarter of the total area in the studied segment of the Chattahoochee, we are not expecting all the phosphorus discharge from them to be easily eliminated. We therefore assume that 10%-15% of the total nonpoint source loads, some 20-30 tonnes per year, mainly from agricultural sources, can be easily reduced by certain types of control strategy. This determines the maximum size of the potential trading market. In the following quantitative uncertainty analysis, the possible load reduction for agricultural sources is parameterized as R_L, which is distributed within a range of (20, 30) tonnes per year.

Table 7-1 shows that the percentage of nutrient removal is very different for different BMP strategies, and even for same type of BMP, performance can vary greatly. The actual effect varies greatly. The actual effect of a BMP is a function of site characteristics, such as the type of tillage, vegetation, soil, slope and local management strategy. Performance should be derived from quantitative analysis, such as some research with the models of HSPF and SWAT, at the plot-scale, to estimate the water quality response on BMPs (Arabi et al. 2007).

The significant uncertainty involved in the effectiveness of BMPs is regarded as another major uncertainty source, and will be incorporated in the simulation framework. The summary of earlier research has implied that here, when we try to account for the uncertainty in pollution reduction at nonpoint sources, we have to assign a rather broad range to this. Depending on the numbers listed Table 7-1, we will assume the actual effectiveness of BMP implementation in this watershed has a variation between 20% to 100%, which means, if a BMP project is designed to remove 10 kg phosphorus per year, due to the variation of actual performance the phosphorus load reduced will range from 2 to 10 kg/year. The effectiveness rate is also considered as an uncertain parameter, represented by R_B, with a distribution range of (0.2, 1).

7.4.3 Trading ratio

The trading ratio is a very significant factor in determining the outcome of water quality trading and attainment of the environmental and economic targets. Thus choosing an appropriate value of the trading ratio will be an important technical task for the design of trading programs (EPA 2008c). Our exploration on the trading ratio starts with the summary of past researches. Actually used trading ratio values for dozens of projects are listed in Table 7-2(Environomics 1999;

O'Grady and Wilson 2000; Palace et al. 1998). This summary shows that for a water quality trading program that involves both point and nonpoint source dischargers, the value of the trading ratio is normally set between 1.2 to 4. Thus in our analysis framework here, we suppose that the operational parameter of the trading ratio can be varying in the range of (1, 4).

The selection of the trading ratio value is very important for water quality trading programs. It determines how much tradable (saleable) credit can be produced (to pollute elsewhere) from the implementation of a pollution control effort by credit generators. For example, if a stakeholder, say a cattle yard, has built a manure-collecting and processing system to reduce 100 kg/year phosphorus from its pollution load into the river, when the trading program employs a trading ratio of 2.5:1, the stakeholder will have 40 kg/year of phosphorus discharge credit to sell in the trading market. This example also tells us that the higher trading ratio, the lower the credit will be produced by a given pollution management practice.

7.5 Economic analysis

The foundations of trading are that a water quality goal is established and that sources within the watershed have significantly different costs for achieving comparable levels of pollution control. After the water quality target has been established (as in Chapter 6), the next task will be an economic analysis for evaluation of the financial benefit to be derived from the trading program. The constituents of the economic sector, mainly those of the pollution abatement cost and market transaction cost, will be first be discussed, including their associated uncertainty. Discussion of the analysis of the total economic profit of the potential trading market then follows.

7.5.1 Cost analysis for point sources dischargers

The financial attractiveness of trading highly depends upon the relative costs of treatment and pollution costs for pollution sources. A primary step in predicting the feasibility of water quality trading is to estimate point source treatment costs. In a previous substantial piece of research (Jiang et al. 2005), the costs for wastewater treatment for phosphorus removal in Georgia have been analyzed extensively. For upgraded levels of phosphorus treatment, the costs, including the constructing capital cost and operations and maintenance costs, of both entirely new wastewater treatment facilities and adapted existing facilities, have been computed.

By means of a simulation study of the wastewater treatment plant with the same WEST platform as used in Chapter 5, three different strategic alternatives of treatment plant designs, the activated sludge process with alum addition (AS/AL), Anoxic/Oxic (A/O), and Anaerobic/Anoxic/Oxic (A/A/O) configuration for the bioreactor, are considered. This research has shown that the cost of nutrient removal for wastewater treatment plants is highly dependent on plant capacity, the adopted treatment processes, and limit of the effluent concentration. Figures 7-1 and 7-2 show the unit phosphorus removal cost againest the variation of effluent concentration limit. These data come from the report of previous research (Jiang et al. 2005). The cost curve of the (A/A/O) process is not displayed here because it is similar to the figure for the (A/O) strategy. Curve colors represent the different capacities of the wastewater treatment plants.

We can conclude from Figures 7-1 and 7-2 that the method of chemical addition is the most economically effective for the conditions considered. Larger plants have a lower cost to remove a unit amount of nutrient load, and there is an obvious cost increment as the effluent limit becomes more stringent. The results indicate a sharp change in abatement costs between plant capacities of 1 and 10 MGD. We therefore consider that phosphorus treatment in small plants is not cost-effective. It would be better for all the phosphorus removal for point sources to be achieved in those plants with a capacity between 10 and 100 MGD. Recalling from the Chapter 6 that we have suggested an effluent limit of 0.35 mg/L for point sources in this watershed, we consider the cost of phosphorus removal should be generally be between 75 and 105 $/kg. Variation across this range acknowledges the role of uncertainty. Cost of phosphorus removal in WWTP is parameterized as C_P, furthering our subsequent economic analysis of the trading market.

7.5.2 Cost analysis for nonpoint sources pollution abatement

In contrast, the estimated costs to reduce phosphorous in nonpoint sources, especially for the agricultural sources, are often considered to be in a much lower range than for point sources, However, this is not always the case. In fact, some existing projects have been initiated only to find that the cost difference was not as great as originally expected. Therefore, it is important to analyze these costs in order to evaluate the economic incentive for establishing a trading market. A broad range of practices is included for control of the nonpoint sources. The real cost of implementing the BMPs depends on site-specific factors. We have summarized the estimates obtained from several parallel studies and listed them in Table 7-3.

The variations in phosphorus reduction costs are huge. Since there is not a specific investigation on the cost of BMP construction and operation in Chattahoochee watershed, we will continue to employ the conservative strategy for uncertainty analysis, assigning a broad range of variation range for the parameter of NPS phosphorus abatement cost (C_{NP}), depending on literature references. The range of 10-60 \$/kg (4.5-27 \$/lbs) is chosen for C_{NP} for further quantitative analysis.

7.5.3 Transaction cost

Transaction costs also influence the financial attractiveness of any water quality trading program and should be duly considered. These costs represent all the resources needed to implement the trade, including information gathering, market development, negotiation, trade execution, and monitoring. It is not a negligible item in practical environmental management. For example, the cost of water quality monitoring to support the development of TMDLs in the U.S. was approximately as high as \$17 million for the year of 2000 (EPA 2001b).

A rather high transaction cost is often encountered in trading programs, especially when nonpoint sources are included. High transaction costs can produce substantial overall market “friction”. The higher and more variable (uncertain) transaction costs will produce substantial market friction and significantly affect, even diminish, the financial attractiveness of an otherwise effective trade (Boyd et al. 2004; Woodward and Kaiser 2002).

The transaction cost of the water quality trading market depends on such factors as the volume of trading, the program infrastructure used to facilitate trading, and the number and types of participants involved. Previous studies demonstrate significant difference in administration costs across different types of policies to reduce watershed phosphorous pollution (mainly for agricultural nonpoint sources), with a range from 4% to 12 % of the total costs (Carpentier et al. 1998; McCann and Easter 1999). Considering water quality trading is normally accompanied by relatively higher transaction costs than other watershed pollution control policies, we assume herein that the possible transaction costs are proportional to the magnitude of the trading market, with a rate, denoted by *R_Ct*, valued between 10% and 20%. That is, for any single transaction of 1000 dollars, the transaction cost will be between 100 to 200 dollars.

7.5.4 Evaluating the financial profit

In order to explore the financial effectiveness of water quality trading in this watershed, a direct path is to calculate whether a net economic profit will be generated by the trading market. For this purpose, we will try to evaluate the total economic surplus (sum of producer surplus and consumer surplus) of the potential market. Total economic surplus is the primary measure used in welfare economics to evaluate the efficiency of a proposed policy. It is a quite suitable index for the task of predicting the financial effectiveness of the policy of water quality trading. In the market equilibrium model for normal commodities, where the supply curve is increasing and demand curve is decreasing, the total economic surplus is calculated as the area between supply and demand curves to the left of the equilibrium point, denoted by the red and blue color area in Figure 7-3.

As far as the water quality trading market is concerned, its addressed commodity is the phosphorus discharge credit (surplus permit), which is produced from the pollution reduction efforts and will be purchased by the parties facing higher control costs. We begin by generating the supply curve of this market based on the analysis of the producer side. Because the cost of phosphorus reduction varies by the individual source, and the quantity of a product supplied by producers will increase with the higher market price of the product, i.e., with the increase of phosphorus credit prices, more stakeholders will want to participate in the trading program, achieve some extra pollution reductions and sell the so produced credit in the market. Their collective behavior reflected in the trading market will be a downwards-sloping aggregate supply curve.

In addition, due to the involvement of the trading ratio, this credit supply curve is *TR* times higher than the cost curve of the nonpoint sources discharger. For example, if one livestock yard (stakeholder A) faces a cost of 20 $/kg for phosphorus reduction, with a trading ratio of 2:1, he/she can only produce and sell 1 kilogram of credit after he makes a reduction of 2 kilograms, Thus, A will not enter the market unless the credit price is higher than 40 $/kg. Figure 7-4 makes a schematic illustration of the market supply curve of the discharge credit.

Due to the uncertainty involved in the estimation of phosphorus abatement costs and the choice of trading ratio value, the position and shape of this curve will definitely change. In order to reflect the fact that the sources in this watershed have different costs, we further substitute the parameter of C_{NP} with a range between C_{NP}_d, and C_{NP}_u, which respectively represents the minimum and maximum phosphorus abatement costs for nonpoint sources. We suppose the market supply curve is a straight line between these two values.

Next, we will discuss the side of the consumer, in order to determine the demand curve of the trading market. The point sources who face the relatively higher phosphorus removal costs are the potential buyers in the trading market. Theoretically, if the price of the pollutant discharge credit in the trading market is lower than the costs of one discharger, he/she will choose to purchase the discharge permit from market instead of installing treatment on his/her own source. The lower the credit price in the market, the more the point–source owners are willing to participate and the total demand for credits will be higher. The aggregate market demand curve normally has a downward-sloping pattern, as shown in the Figure 7-5.

The market demand curve has a smaller slope than the supply curve due to the fact that the difference in pollution abatement costs for the point sources are varying less than that of the producers side, i.e., nonpoint sources. We also use two parameters here, C_P_d, and C_P_u, which are the minimum and maximum phosphorus removal costs for the point sources, and a straight line between them to simulate the aggregate demand curve of this Chattahoochee watershed water quality trading market.

Based on the above analysis, we are ready to construct the equilibrium market model to calculate the total economic surplus, to examine the financial profit of the potential trading market. An example is illustrated Figure 7-6. In this example, the total economic surplus of this trading market corresponds to the area between the red and blue solid lines to the left of the equilibrium point (Q_E, P_E). Mathematically, it is calculated by:

$$S_{TM} = \int_0^{Q_E} \left(C_P - P_{Credit}\right) dQ - R_{Ct} \cdot P_E \cdot Q_E \qquad (7\text{-}1)$$

In the above equations, S_{TM} is the total market surplus of the potential market; C_P is the cost of phosphorus removal by waste water treatment plants in this watershed, which is considered to be equal to the price they are willing to pay on the trading market; P_E and Q_E are respectively price and quantity for in the market; P_{Credit} is the price of discharge credit in the trading market, which is determined by the cost of phosphorus abatement for nonpoint sources, calculated by

$$P_{Credit} = C_{NP} / TR \qquad (7\text{-}2)$$

where C_{NP} is the cost of phosphorus reduction at nonpoint sources and TR is the trading ratio employed in the trading program.

Note that the demand and supply curve is only one of multiple possible scenarios. Because substantial uncertainty exists throughout every detailed part of the water quality trading program, the positions and shapes of these two curves will change significantly when we evaluate it under uncertainty. As a result, when we estimate the total economic surplus, the resulting uncertainty has a substantial influence on it. Sometimes no market surplus is generated as an incentive for either the producer or the consumer of the credits, because the supply curve is located entirely above the demand curve. For this, we say there is no financial attractiveness for water quality trading under such conditions.

7.6 Integrated evaluation system

So far, for the foregoing discussion of this chapter and that of Chapter 6, we have evaluated these major factors that are uncertain and have a substantial impact on the effectiveness of water quality trading policy, from both environmental and economic perspectives. We will now couple these two parts together and construct a rather broad integrated computational system to assess this policy from the two perspectives jointly, in order to achieve a comprehensive and scientific evaluation of the water quality trading in the Chattahoochee watershed.

Figure 7-7 illustrates the major components in this procedure and the relations between them. The arrows in this figure mean that one constituent or factor in the system is used to calculate the other.

This integrated system has two principal parts to it, which correspond to the dual targets of water quality trading (and similar environmental management practices), which interact with each other. The comprehensive watershed simulation system constructed in Chapter 5 and 6 is employed as one part here (for watershed and water quality evaluations), and the economic analysis component is the other, for assessing the financial profit of the trading market.

The computational procedures demonstrated in Figure 7-7 work in such a way: first, a trading market is supposed to exist in this watershed and the status of this market, its scale (participants and trading volumes) and the price of phosphorus discharge credits are collectively determined by both sides of the demand and supply, as well as transaction costs. Based on the market equilibrium model, the total economic surplus is calculated, as an index to show the financial benefit produced by this water quality trading market. Sometimes the market may not generate an economic surplus, which means it is not economically effective and will not lead to any transaction happen. For these cases, the economic surplus is zero.

Next, we will examine the environmental impact induced by this trading market. As a consequence of trading transactions, credit buyers will discharge an extra amount beyond their original permits, while sellers are supposed to discharge less. Uncertainty is substantially involved in the process of the pollutant offset, both in the amount and location, and maybe its timing too. Our watershed simulation system is employed again to evaluate the subsequent total pollution load and instream water quality, and how they might respond, if trading were implemented, and whether trading will meet the predefined environmental targets, all under uncertainty.

This integrated evaluation system principally generates two outcomes: the total market surplus and river water quality. These two items are exactly suitable for assessing the trading policy, according to the dual targets. When we need to evaluate whether a candidate trading scheme will lead to expected targets for a certain watershed, we can simply feed the information into the above system, and examine the resulting outputs. Based on the analysis of all the sources that will brought uncertainty into the trading programs, a sampling-based framework is again used for assessing candidate trading schemes in the presence of all the sources of uncertainty involved.

7.7 Analyzing the uncertainty and sensitivity

7.7.1 Sampling-based method

Having thus identified uncertain factors involved in water quality trading, which of them, we ask, are most critical in determining the efficacy of trading programs? More specifically, after we have composed a framework to evaluate such a policy, which component or factor has the most significant (conditional) sensitivity?

Here we continue to employ the sampling-based method to account for the uncertainty. In order to elucidate the propagation of uncertainties in the WQT evaluation system, the entire system is embedded in IMUSEM. In other words, we input all the parameters and their associated uncertainty (listed in the Table 7-4) into the simulation system, to predict the financial and environmental consequences thereof, and reveal the attaching parametric sensitivity.

Based on the assessment of the uncertainties associated which each category of constituent factors, a parametric set with the size of 1000 points are randomly sampled according to the prior distribution ranges, which are listed in the Table 7-4, and fed into the water quality evaluation system for computation. Due to the propagation of these significant uncertainties, the distributions of water quality and economic surplus results are also rather scattered.

7.7.2 Behavioral classification

The approach of the RSA is applied in a particular way for handling the uncertainties for aiding the water quality trading program development. Thus, the definition of behavioral simulations is made according to the main targets of water quality trading programs, which are: to achieving both water quality improvement and a net financial benefit. The no-trading conditions are taken as the baseline for screening the favorable system behaviors. That is, if the post-trading water quality is better then the original conditions without trading, and the proposed trading market can produce a positive profit, we will say this trading policy is valid, or feasible, in principle.

In particular, since we have calculated a TMDL in the previous chapter, we will employ it as the baseline for evaluating water quality equivalence. The results of this environmental-economic system are conditioned as follows: if the simulated total pollution load is less than 330 tonnes per year and the total economic surplus is larger than zero, this is classified as a behavioral set, which reflects a valid and effective trading policy; otherwise the simulation will be classified into the nonbehavioral set. This RSA framework is illustrated in the Figure 7-8.

Computational results show that 450 simulations (and associated parametric vectors) out of 1000 in total are finally classified into the behavioral set. These “valid” simulations are considered to be able to provide positive results of trading program. Based on them, the most promising (and feasible) trading scheme can then be suggested.

7.7.3 Result

RSA is used here to answer the questions such as: which uncertain factor is most significant in determining whether the water quality trading programs can attain the expected performance, and under what condition the trading market will be more effective? Conditioned by the designated environmental and financial requirements, or targets of water quality trading programs, the significance of each uncertain factor, from both the technical basis and the policy perspective are thereby quantitatively revealed by the application of RSA method. Table 7-5 lists the calculated values of the standard K-S statistic Z for each parameter, as an index to represent the regionalized sensitivity.

These results show that the minimum phosphorus reduction cost of nonpoint sources C_{NP}_d is the most important factor in this system, followed by N_C, N_L, C_{NP}_u, R_B, TR, and C_P_u, while the other parameters are not very sensitive. We generally see from this result that parameters associated with nonpoint sources are all ranked highly, which might imply that the success of any water quality trading program in the Chattahoochee watershed will be highly dependent on the characteristics of the nonpoint sources. We are therefore curious about how this dependency happens, in order to find how these factors can be manipulated to improve the reliability of the proposed programs and to facilitate the wider application of trading policies.

Taking the parameter of C_{NP}_d as an example, Figure 7-9 displays the influence of the joint actions of C_{NP}_d and the trading ratio on the RSA classification results. The blue circles in the figure are the behavioral data points and the red circles are belong to the nonbehavioral set. We coarsely see from the figure that, if C_{NP}_d and TR are both high (top right corner), this leads to a nonbehavioral point. With a lower C_{NP}_d value (bottom part) the occurrence of a behavioral point is much more frequent than that when C_{NP}_d is high. In other words, when the pollution control cost of nonpoint sources is highm the trading program will be very probably ineffective, especially when a high value of trading ratio is employed. The response to different trading ratio selections will be later discussed in depth.

In addition, if we want reduce the uncertainty to enable the trading to be more applicable in the future, a number of approaches can be used to reduce or compensate for the uncertainties, such as surveys for more and accurate information, monitoring to verify load and load reductions, refining the simulation tool to reveal system behavior, or adoption of better uncertainty processing techniques. Based on the RSA, better investigation of the watershed nonpoint sources, tracking and evaluating their discharge amounts, their possible reductions, and their abatement costs, will increase the feasibility of water quality trading most significantly.

7.7.4 Decision support under uncertainty

The procedures of simulation and the attaching capacity for the analysis of uncertainty provide the platform on which we have been constructing our evaluation of candidate pollutant trading schemes for managing water quality in a watershed. In order to support decision making in water quality management, in our RSA framework, the form of trading market (such as size, participants, credits available for trading) and trading ratio are all considered as decision parameters, and in combination with all the other uncertainty sources, this framework is able to identify what kind of trading design will more likely be maximally robust to make the program of water quality trading successfully realized in spite of uncertainty.

Through the application of the computational framework, the behavioral values for the management parameters are generated. Obviously, these values have more probability for leading to successful trading programs. However, given the highly nonlinear property of the economic-environmental system, the behavioral and nonbehavioral sets are quite widely scattered, and interspersed with each other. The "optimal" values for the decision parameters cannot therefore be identified by this framework directly.

Using the trading ratio as an example, we illustrate how the integrated evaluation framework will aid the decision process. Identifying the optimal trading ratio is one important quantitative task in designing the pollutant trading scheme. So the question becomes: at what trading ratio will trading become more likely (for the reliability of water quality trading programs) to generate higher (for policy effectiveness) water quality improvement and economic benefit?

The selection of a trading ratio reflects a "trade-off" relation between environmental benefit and economic profits. Simply speaking, with a lower trading ratio of NPS to PS, say 1:1, the financial benefit is produced only if the control cost of nonpoint sources is less than that of the point sources, but zero environmental improvement will be generated. However, if the trading ratio is 4:1, then the trading will not happen (no financial benefit produced) unless the control cost of nonpoint sources is less than a quarter of that of the point sources. But once this happens, it leads to environmental improvements. This is realistic considering that the U.S. EPA's Draft Framework for Watershed-Based Trading cautions against using ratios that are too stringent and those that eliminate the economic benefits of trading (Environomics 1999).

We have plotted the trading ratio versus our evaluation indexes, total economic surplus and total phosphorus load, to reveal the relation between them. First, Figure 7-10 shows the value of the total economic surplus of the trading market versus the trading ratio for all the model realizations, including both behavioral (marked as blue circles) and nonbehavioral (marked as red circles) sets. It tells us if the trading ratio is chosen to be low, the positive financial benefit is very likely to occur, but when the trading ratio is set as a relative high value, larger than 2, there are more chances that it will lead to market inefficacy, and no transaction is implemented.

From Figure 7-10 we see that a large portion of the simulations generate a positive economic surplus and only a few of them (25.6 %) will lead to financial ineffectiveness. This is dependent on our prior evaluation of the parametric variations for the specific conditions of the Chattahoochee watershed, in particular, the costs of reducing phosphorus , which range from $75 to $105 per kilogram for the point sources relative to the range of $10 to $60 per kilogram for the various agricultural management practices for controlling nonpoint sources.

Figure 7-10 also shows that the trading ratio is such an important factor for determining whether economic benefits can be produced by trading. A too high (stringent) value could eliminate the financial incentives for trading. In this case, if the trading ratio is less than 1.5, then the financial benefit will surely be positive despite all such uncertainties. However, this is not all we want, because we see many red dot (means either of the dual criteria is not achieved) are still located in the left part of Figure 7-10.

Regarding the other target of water quality improvement, the response of total pollution load amount to trading ratio values is demonstrated in Figure 7-11. In this figure, blue and red circles represent the behavioral and nonbehavioral simulations, and the pink solid line, which is horizontal with the value of 330 tonnes per year, is the environmental baseline (or cap) imposed by the TMDL. In other words, without the trading program implemented, the watershed pollution load regulated by TMDL averages 330 tonnes per year.

After the trading market is constructed and functions, the load amount will be changed because pollutant discharge offset happens both spatially and quantitatively. In order to track the relationship of these two items in Figure7-11, we derive a trend line from the total simulation set (including both red and blue circles) by means of a simple second-order polynomial regression, which is shown by the green solid curve. The trend line depicts a general pattern of the response of phosphorus load to the varied value of the trading ratio. If we compare it with the pink curve, which can be regarded as the trend line of no-trading conditions, we can conclude that when trading ratio is larger than 1.5 the trading program will be more likely to result in water quality improvement, in spite of all the uncertainties.

Another interesting implication of this trend line (greed solid curve in Figure 7-11) is that it does not continue only to decrease as the trading ratio increases. Inflexion happens when the ratio is approximately three. After the inflexion, the green line switches from departing away from, to approaching the pink line. The interpretation for this phenomenon could be that when the trading ratio becomes very high, the trading market shrinks due to the function of a market. When a lower volume of pollution credits is traded, the system behavior will be more similar to that with no-trading conditions. Recalling Figures 7-6 which describes the figure trading market equilibrium given market supply curves, the supply curve will shift up when the trading ratio increases, and then the trading volume decreases and the total economic surplus diminishes. Figure 7-12 show the relation between trading volume in market and variation of the trading ratio.

This finding challenges the consensus of a rigid “trade-off” relation between water quality improvement and market financial profit in the case of water quality trading. For this case, if we compare trading ratios between 3 and 4, it is seemingly reasonable that the trading ratio of 4 should lead to more environmental benefit than when 3 is used. But our integrated evaluation gives the contrary result. With the consideration of the magnitude of trading market, the computational results shown in Figure 7-11 demonstrate that in this case we can say the value of 3 will be more like to lead to greater environmental improvement.

For identifying the acceptable value for the trading ratio based on our integrated framework, we suggest the value of 3.0 for the Chattahoochee watershed for potential water quality trading programs, given our evaluations on the factors and associated uncertainty. For better illustrating the environmental consequence of a functioning water quality trading market, again taking the typical hydrological year of 1995 as an example, we have plotted in Figures 7-13 and 7-14 the daily time series of instream phosphorus concentration and watershed phosphorus load into Lake

West Point. A comparison between with trading markets and the original conditions without trading (but water quality is assured by the rigid policy of the TMDL, as discussed in Chapter 6) is demonstrated. The simulation results for without-trading scenario are from the same computation in Chapter 6, as what is shown by Figures 6-8 and 6-9. The with-trading scenario is simulated with every parameter are set as the median value in Table 7-4 and the trading ratio (*TR*) is set as 3.0. Figures 7-13 and 7-14 show the environmental benefit resulted from the operation of a trading market. According to these two figures, further water quality improvement will be achieved with the transactions of pollutant discharges between point and nonpoint sources suggested in this study, at the same time, both buyer and seller in the trading market gain a certainty amount of financial profit.

7.8 Summary

In this chapter, we have applied IMUSEM to comprehensively explore the policy of water quality trading in the presence of various sources of uncertainties. The computational results have generally shown that water quality trading is a very feasible policy to be implemented in this watershed, because we are taking rather conservative assumptions when defining the magnitude of the involved uncertainty, and the simulation results demonstrate that if the trading ratio is set appropriately, the trading market will very likely to generate both positive environmental and financial benefits.

The results of the RSA algorithm indicate that the cost of nonpoint source reduction (through BMPs) has the highest sensitivity in determining the success of trading programs, so that we will conclude that, if for a watershed the costs of construction and operation of BMPs are relatively low, then water quality trading will be more likely to be effective. This also implies that if we can attain more accurate information on BMP costs, we can get a more proper evaluation of the efficiency of potential trading markets. For this case, the fluvial parameters are least sensitive, which means that the delivery of phosphorus along the channel is not an important process. One reason might be that our concerned pollutant, total phosphorus, is relative conservative in the main stem of the river channel, but for other constituents such as BOD, the channel process, and thus the locations of the trading participants, will be more important.

The results of this case study also suggest that the financial benefit to be generated by a water quality trading market will be somewhat lower than original expectations. This point is consistent with the fact that many pilot trading programs have been implemented, but little direct evidence of their successes has been observed. A clear permit system and monitoring system for both point and nonpoint sources are a necessary precondition of trading, but actually in most of the watersheds nonpoint sources are not regulated, and monitoring the nonpoint source itself is a very difficult task.

Considering these difficulties for effectively applying water quality trading, it is more necessary to develop a scientific methodology to design the reliable trading programs. We believe that this framework, modeling with comprehensive consideration of uncertainty, is an appropriate path for this kind of management-support study.

Table 7-1: Estimation of the effectiveness of some BMPs

BMP	Nitrogen removed (%)	Phosphorous removed (%)
Urban storm water management	25-33	20-64
Pasture	20	14
Cattle, swine waste management	80	80
Poultry waste management	14	14
Cover crops	34-51	10-20
Forested buffer	48-65	10-20
Grassed buffer	35-50	53
Resource protection	4-20	25-75
Non-structural cropland	25-76	8-40
Wet pond	13-16	16-43
Wetland basin	39-48	44-63
Bio-filter	17-39	18-46
Media filter	37-48	27-38

Data source: (Palace et al. 1998; WERF 2008)

Table 7-2: A summary of applied trading ratios

Projects	Trading Ratio
Chatfield Reservoir Trading Program	2:1
Cherry Creek Basin Trading Program	1.2 to 3:1
Kalamazoo River Water Quality Trading Demonstration	2 to 4:1
Lake Dillon Trading Program	2:1
Maryland Nutrient Trading Policy	2:1
Minnesota River Nutrient Trading Study	3:1
New York City Watershed Phosphorus Offset Programs	3:1
Rahr Malting Permit Program	2:1
Red Cedar River Pilot Trading Program	2:1
Rock River Basin Pilot Trading Program	2.1 to 3.7:1
Southern Minnesota Beet Sugar Cooperative Plant Permit	2.6:1
Specialty Minerals, Inc. in Town of Adams	2:1
Tar-Pamlico Nutrient Reduction Trading Program	2: to 3:1
Town of Acton Publicly Owned Treatment Works	3:1
Wayland Business Center Treatment Plant Permit	3:1
Wisconsin Effluent Trading Rule Development	2:1
Dillon Reservoir in Colorado	2:1
South Nation River Watershed, Ontario, Canada	4:1

Data source: (Environomics 1999; O'Grady and Wilson 2000; Palace et al. 1998)

Table 7-3: Estimates of costs of phosphorus reduction at nonpoint sources

Location	Cost of phosphorus reduction ($/lb/yr)	Source
General estimation	0.26-5.22	(Czapar et al. 2006)
Lake Erie Watersheds	2.5-40	(Forster and Rausch 2002)
Lower Boise, Idaho	5	(Ross and Associates 2000)
Upper Midwest	6	(Faeth 2000)
Fox-Wolf Basin, Wisconsin	26	(Environomics 1999)
Lower Green Bay, Wisconsin	1.96-30.4	(Schleich and White 1997)
Chesapeake Bay	10	(Camacho 1991)

Table 7-4: Parameters and their prior distribution ranges

ID	Description	Symbol	Lower bound	Upper bound	Unit
1	Predicted extra pollutant discharge	E_L	5	10	tonne/yr
2	Watershed load available for reduction	R_L	10	20	tonne/yr
3	Efficacy of pollution management practice	R_B	0.2	1	--
4	Trading ratio	TR	1	4	--
5	Index of annual hydrological pattern	N_C	1	35	--
6	Upstream reservoir discharge concentration	N_Q	0.01	0.02	mg/L
7	Point source effluent concentration	N_W	0.3	0.35	mg/L
9	Fluvial process parameters	N_F	1	20	--
10	Minimum cost of phosphorus reduction by WWTP	C_{p}_d	75	105	$/kg
11	Maximum cost of phosphorus reduction by WWTP	C_{p}_u	75	105	$/kg
12	Minimum cost of phosphorus control by NPS BMP	C_{np}_d	10	60	$/kg
13	Maximum cost of phosphorus control by NPS BMP	C_{np}_u	10	60	$/kg
14	Transaction cost rate	R_Ct	0.1	0.2	--

Table 7-5: Parametric sensitivity index

Symbol	Z	Rank	Symbol	Z	Rank	Symbol	Z	Rank
N_C	5.18	2	C_P_d	0.48	14	E_L	0.71	12
N_Q	0.86	8	C_P_u	1.50	7	R_L	0.58	13
N_W	0.79	10	C_{NP}_d	5.96	1	R_B	3.54	5
N_L	4.60	3	C_{NP}_u	3.64	4	TR	1.62	6
N_F	0.86	9	R_Ct	0.74	11			

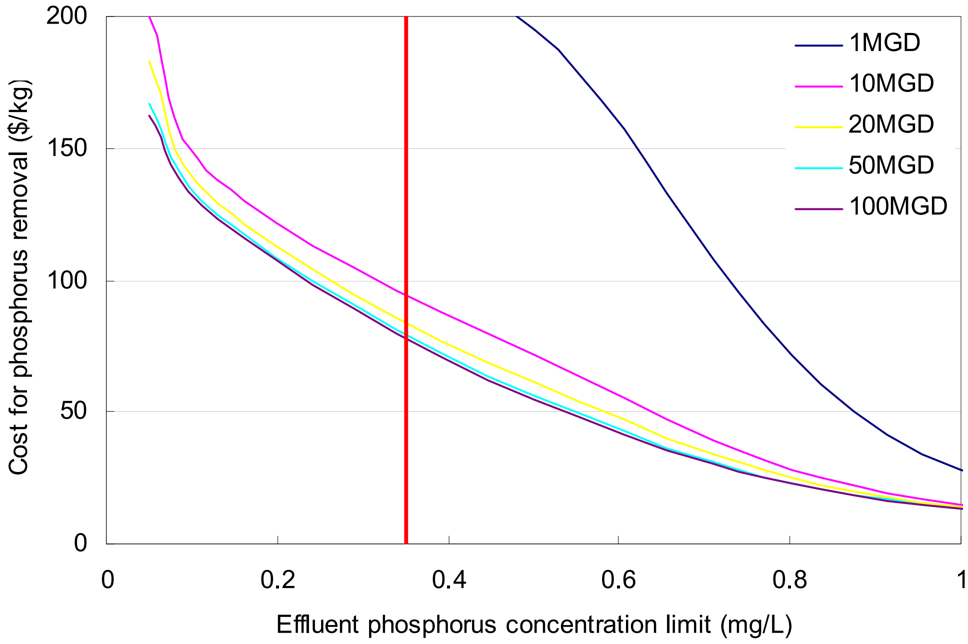


Figure 7-1: Phosphorus removal cost curve (AS/AL)

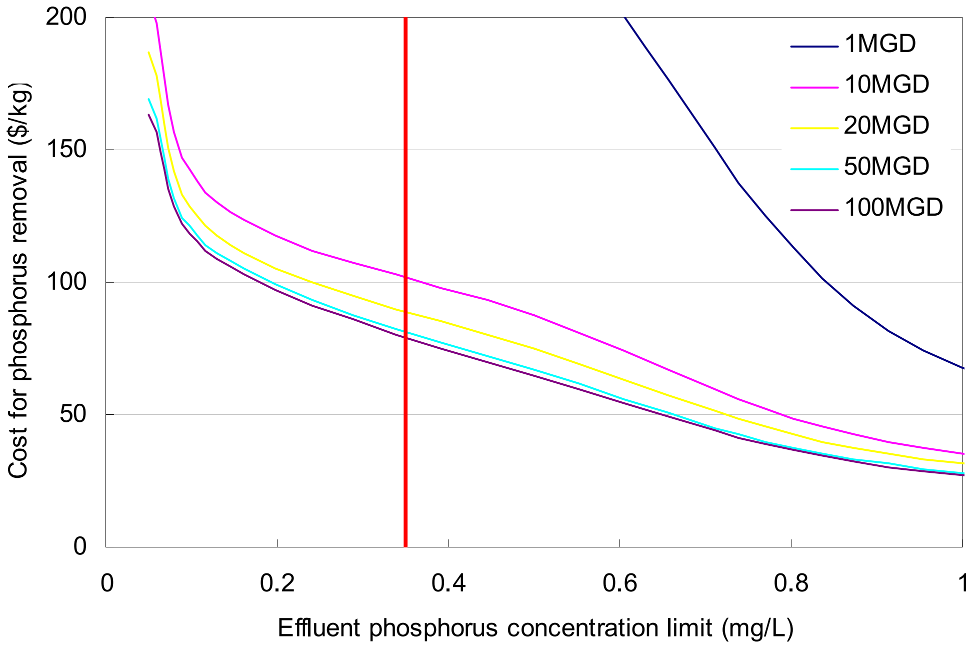


Figure 7-2: Phosphorus removal cost curve (A/O)

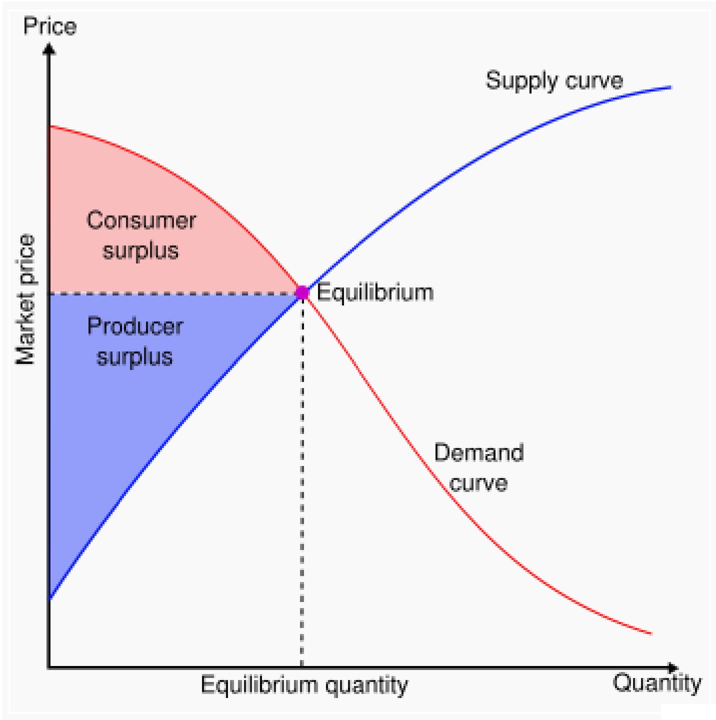


Figure 7-3: Economic surplus of an equilibrium market

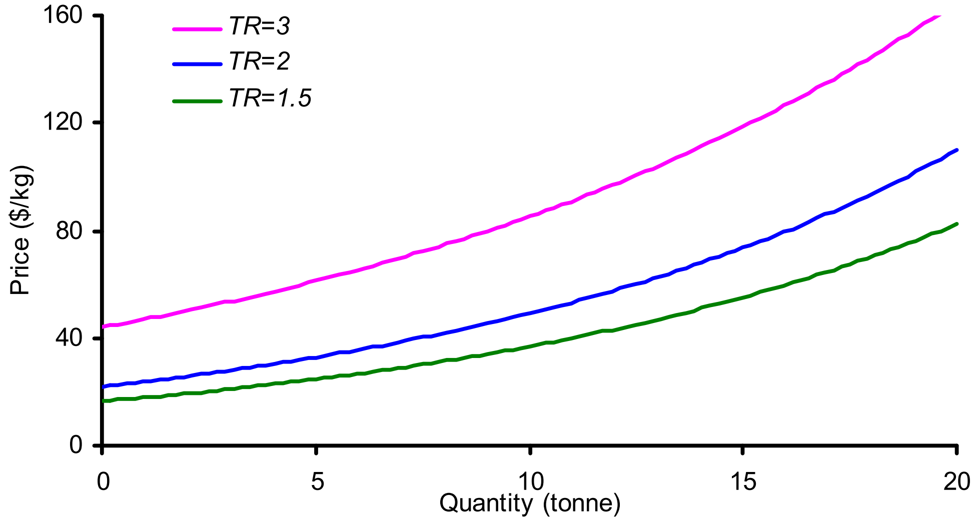


Figure 7-4: Supply curve of phophorus discharge credit

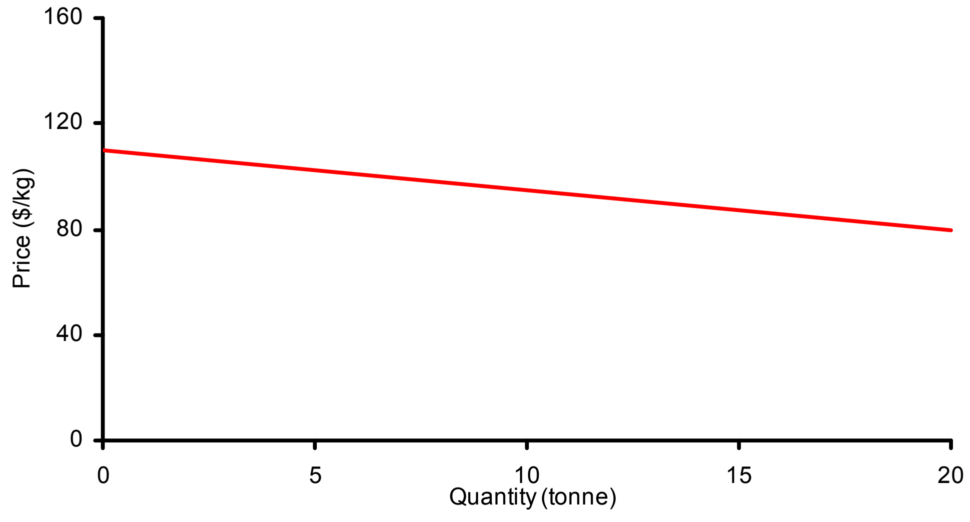


Figure 7-5: Demand curve of phophorus discharge credit

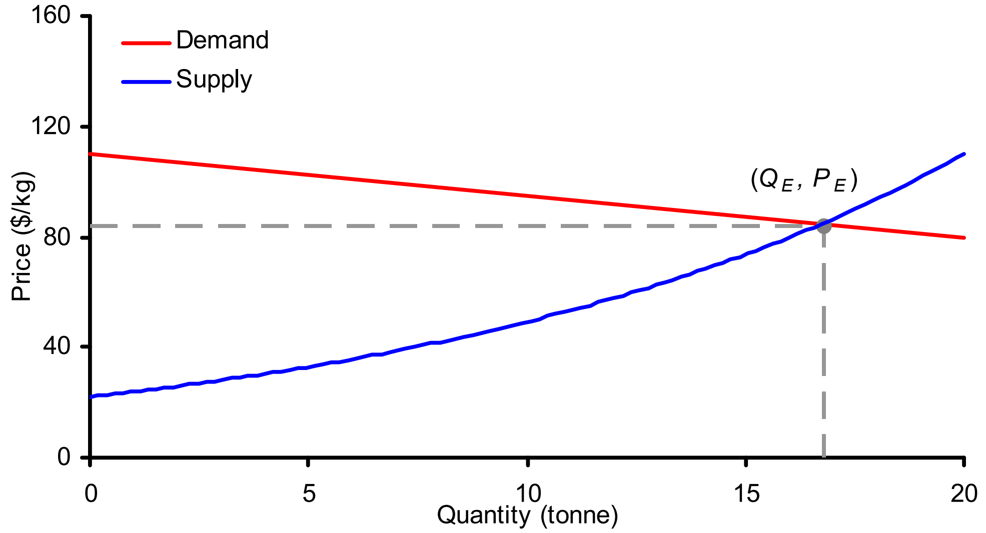


Figure 7-6: Equilibrium water quality trading market

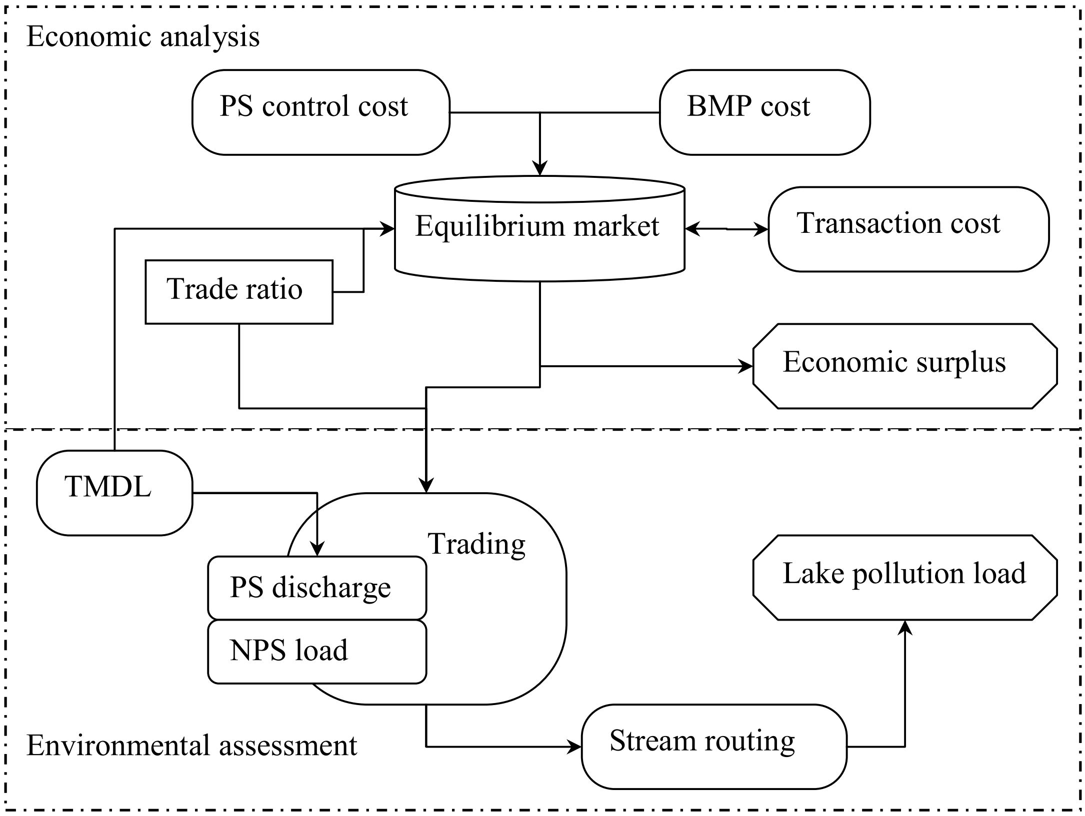


Figure 7-7: Integrated water quality trading evaluation system

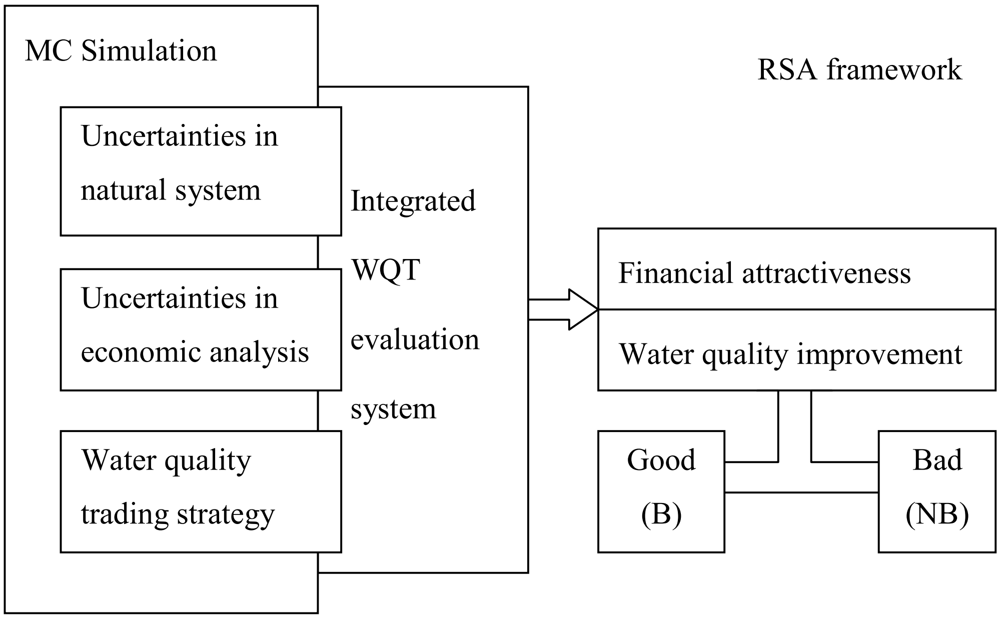


Figure 7-8: RSA framework for evaluating water quality trading

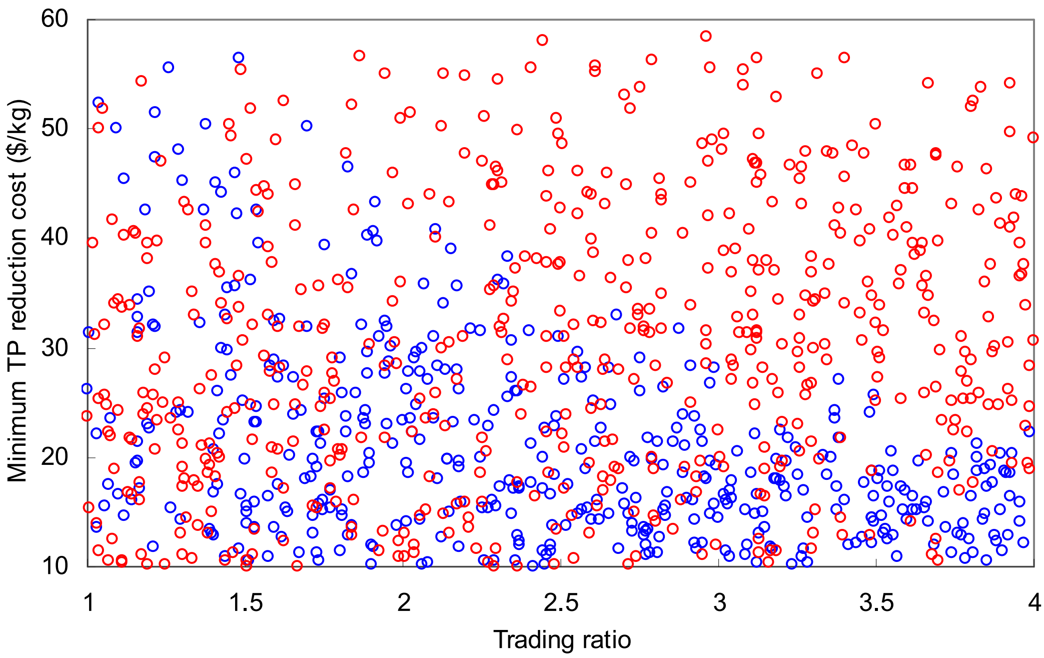


Figure 7-9: Binary classification results for C_{NP} versus TR

(Blue dots are behavioral simulations and red dots are nonbehavioral ones)

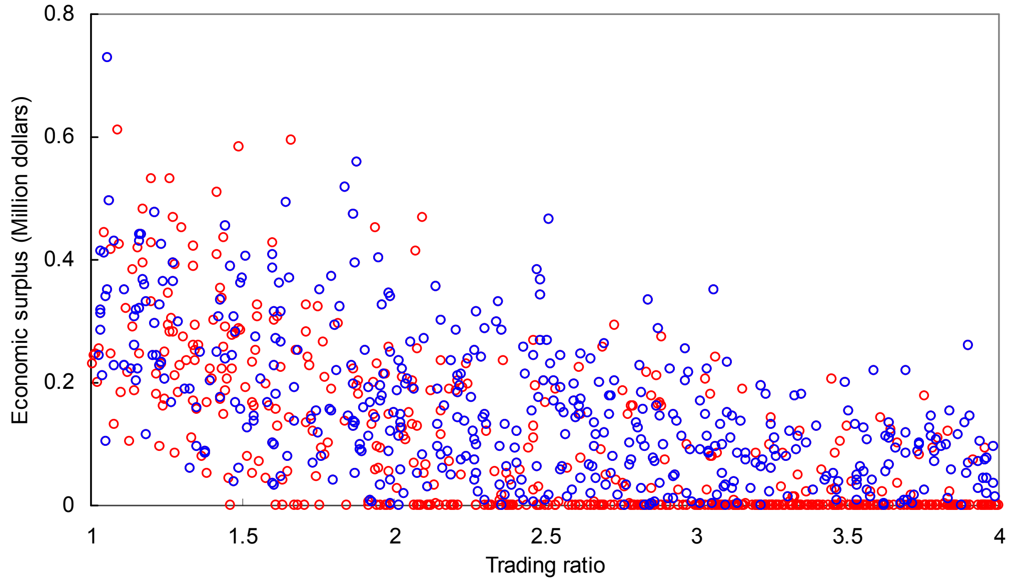


Figure 7-10: Economic surplus vs. trading ratio

(Blue dots are behavioral simulations and red dots are nonbehavioral ones)

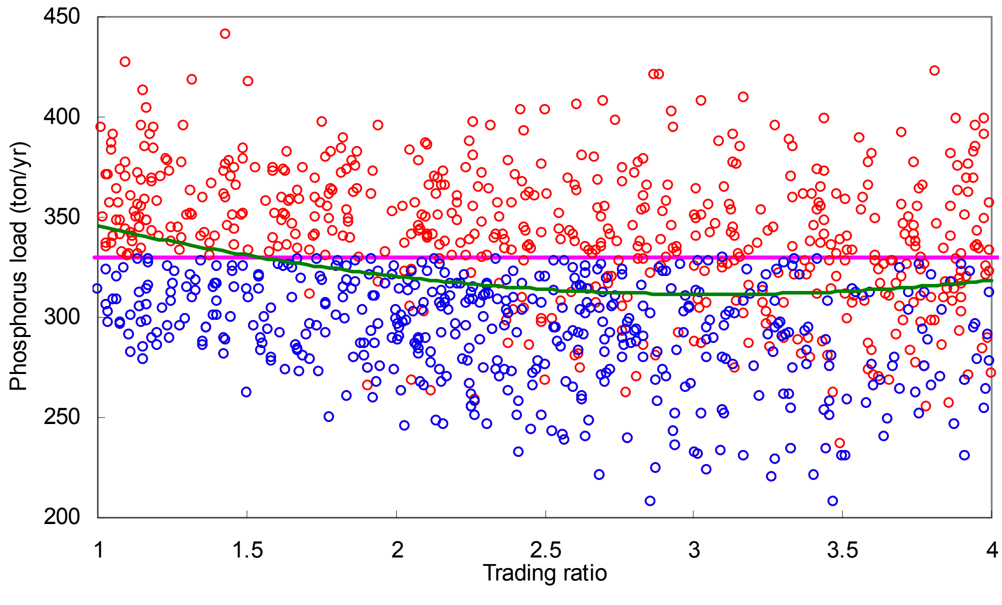


Figure 7-11: Total phosphorus load vs. trading ratio

(Blue dots are behavioral simulations and red dots are nonbehavioral ones)

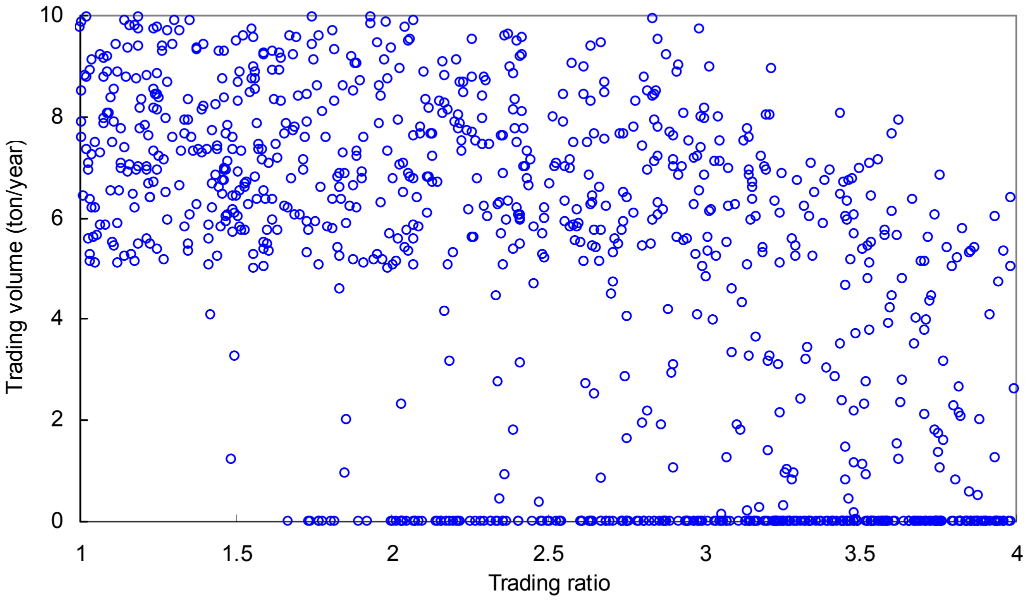


Figure 7-12: Trading volume vs. trading ratio

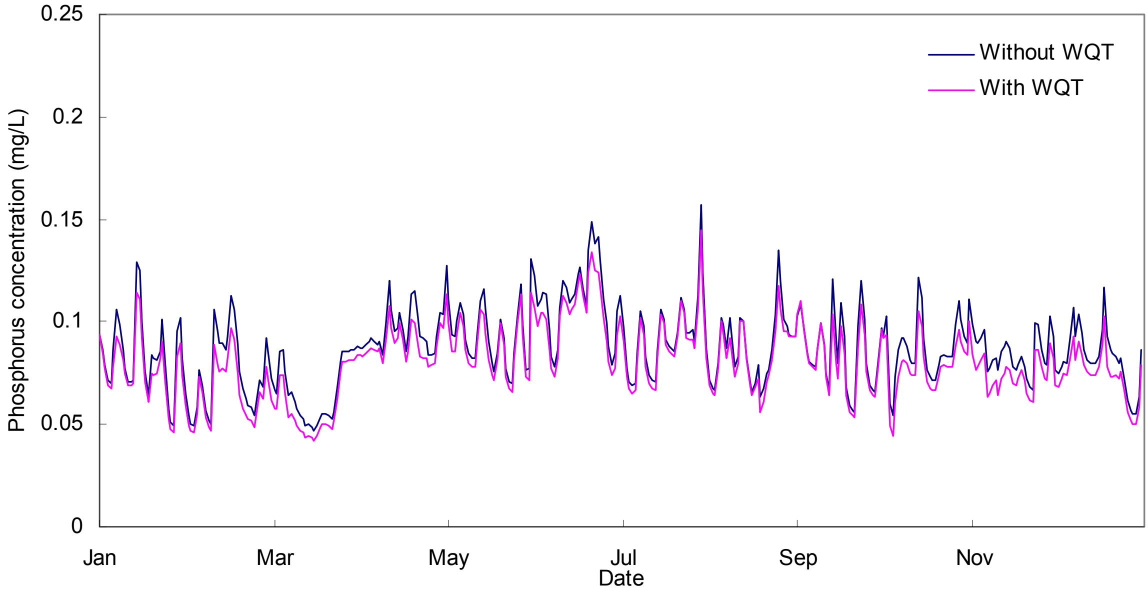


Figure 7-13: Effects of WQT on phosphorus concentration

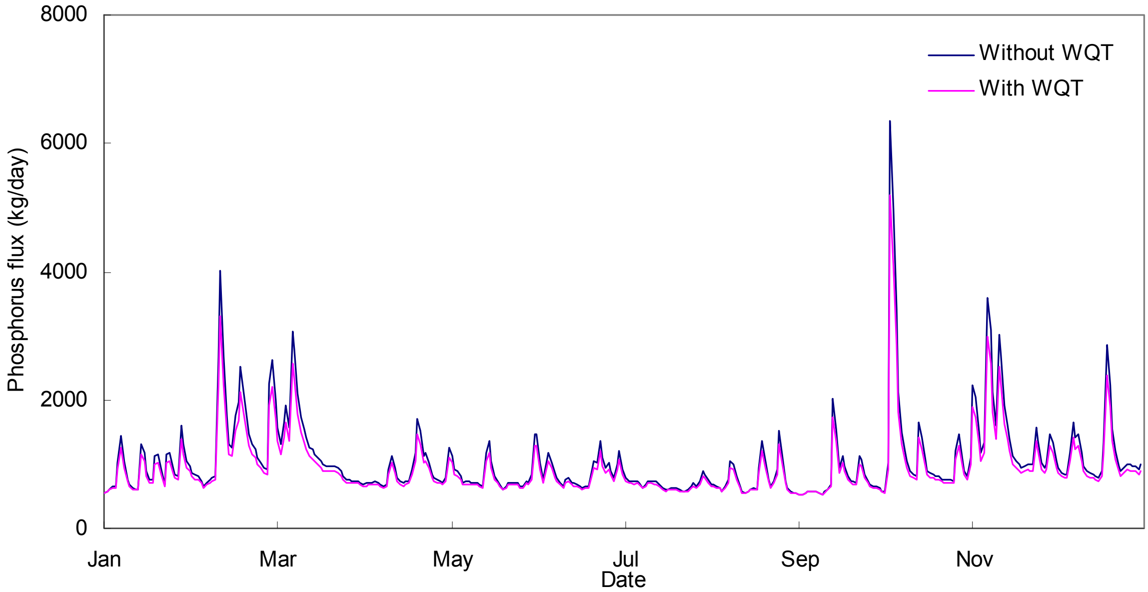


Figure 7-14: Effects of WQT on phosphorus flux

(At inlet of Lake West Point, 1995)

Chapter 8

CONCLUSIONS AND RECOMMENDATIONS

8.1 Discussion and conclusions

Overall, this dissertation has addressed a rather broad topic that covers several major issues in the field of environmental systems analysis. Accordingly, significant contributions achieved by this dissertation are summarized as follows.

(1) In order to better characterize the watershed system for achieving more scientific environmental management, all important sources of uncertainty in the natural system, social-economic factors, and management practices are comprehensively identified and quantitatively expressed within a probabilistic format. A sampling-based approach, such as Monte Carlo simulation, while simple, is yet a powerful tool to account for uncertainties in watershed modeling and management.

(2) For the analysis of uncertainty and sensitivity, the method of regionalized sensitivity analysis is investigated in detail in this study. Its conceptual basis and the numerical stability of a typical RSA-KS algorithm are discussed in depth and suggestions are given for applying it with more reliability. Treatment of the numerical stability of the RSA has in general been overlooked previously. The major objective achieved herein is reviving this method and generalizing it as a standard and universal approach for the task of systems analysis and quality assurance of models.

(3) Paying attention to the Chattahoochee watershed surrounding Atlanta, a comprehensive model system has been assembled to simulate the pollutant behavior of both point- and nonpoint- source discharges, with subsequent instream routing. The part of channel process simulation component is calibrated with sparse monitoring data with a probabilistic algorithm derived from the concept of RSA. This type of integrated watershed simulation system is an appropriate way for studying the water quality problem for a spatial large scale, and it is then used as the engine of the entire uncertainty evaluation and decision-supporting framework.

(4) The assembled watershed simulation system is embedded into the sampling-based framework for assessing the impacts of uncertainty on watershed behavior, and for enabling an analysis of the regionalized sensitivity. These explorations have further promoted our understanding on the watershed and pollutant characteristics, for achieving a solid basis for management and control. With this framework, the distribution and routing of pollutant througthout the entire watershed is identified, with sufficient evaluation on the associated uncertainty. Furthermore, regarding two popular pollution control policies, TMDL and water quality trading, the proposed framework of integrated watershed modeling under uncertainty and this specific case study in Chattahoochee watershed has illustrated a good performance for the tasks of underpinning policy development and assessment.

8.2 Recommendations for further research

The kind of integrated assessment of models and uncertainty proposed and demonstrated in this dissertation is particularly important and useful for supporting environmental policy and management. Based on this study, further research is recommended along the following lines.

(1) The method for uncertainty/sensitivity processing in this dissertation, the RSA-KS algorithm, is essentially a univariate index. It is only able to assess the effect of an individual factor, but cannot detect interaction among several factors, i.e., any parametric dependency or covariance structure inside the model cannot be identified. Thus we have herein often used the scatter plot and correlation coefficient to compensate, but these methods have rather obvious limitations, such as not working well for nonlinear problems. Some experimentation and analysis has been implemented to invent a multi-dimensional index based on the concept of the K-S statistical test, which would reveal such multivariate parametric interaction (Shi 2007). However, the methodology was in the end considered to be not theoretically mature enough and therefore excluded from this dissertation. This would be an obvious target for future research.

(2) Currently (herein), uncertainty in the input factors has been enumerated on the basis of model calibration, former experience and literature references. Since these prior parametric distributions are themselves uncertain, they should be examined and evaluated very carefully. It is suggested that the identification and characterization of all uncertainty sources should be performed jointly by the modeler, the watershed manager, and stakeholders (Refsgaard et al. 2007).

(3) We have attempted to set up an integrated modeling under uncertainty framework for supporting environmental management. Like any new thing, much remains to be improved. For example, integration of the components is rather loose. If we want the proposed framework to be widely used in real management practices, software for this framework (at present only the model is programmed as software) should be a future direction for research. In addition, a web-based publication of these decision-supporting tools, with attractive user-interactive functions, is

considered as a more exciting prospect. In fact, the development of a web-based version of the WWQS model, which can be manipulated by the user through a connection to internet, has been already launched, although this faces many obstacles of both a technical and a design nature.

(4) Finally, application of the proposed systematic framework is expected not to be limited to the assessment of TMDL and water quality trading issues, aiding decision-making. More importantly and significantly, it can be used in the challenge of studying the topic of sustainability, or the exploration of other innovative conceptions, such as the adaptive implementation of management policy, or for the city as a “force for good” in the environment (Beck et al. 2008b). We hope and believe the methodology proposed in this dissertation can make further significant contributions to environmental studies in the near future.

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