ABSTRACT OF DISSERTATION

Mohammad Tufail

The Graduate School

University of Kentucky

2006

OPTIMAL WATER QUALITY MANAGEMENT STRATEGIES FOR URBAN WATERSHEDS USING MACRO-LEVEL SIMULATION MODELS LINKED WITH EVOLUTIONARY ALGORITHMS

ABSTRACT OF DISSERTATION

A dissertation submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy in Civil Engineering
at the University of Kentucky

By

Mohammad Tufail

Lexington, Kentucky

Director: Dr. Lindell E. Ormsbee, Professor of Civil Engineering

Lexington, Kentucky

2006

ABSTRACT OF DISSERTATION

OPTIMAL WATER QUALITY MANAGEMENT STRATEGIES FOR URBAN WATERSHEDS USING MACRO-LEVEL SIMULATION MODELS LINKED WITH EVOLUTIONARY ALGORITHMS

Urban watershed management poses a very challenging problem due to the various sources of pollution and there is a need to develop optimal management models that can facilitate the process of identifying optimal water quality management strategies. A screening level, comprehensive, and integrated computational methodology is developed for the management of point and non-point sources of pollution in urban watersheds. The methodology is based on linking macro-level water quality simulation models with efficient nonlinear constrained optimization methods for urban watershed management. The use of macro-level simulation models in lieu of the traditional and complex deductive simulation models is investigated in the optimal management framework for urban watersheds. Two different types of macro-level simulation models are investigated for application to watershed pollution problems namely explicit inductive models and simplified deductive models. Three different types of inductive modeling techniques are used to develop macro-level simulation models ranging from simple regression methods to more complex and nonlinear methods such as artificial neural networks and genetic functions. A new genetic algorithm (GA) based technique of inductive model construction called Fixed Functional Set Genetic Algorithm (FFSGA) is developed and used in the development of macro-level simulation models. A novel simplified deductive model approach is developed for modeling the response of dissolved oxygen in urban streams impaired by point and non-point sources of pollution. The utility of this inverse loading model in an optimal management framework for urban watersheds is investigated.

In the context of the optimization methods, the research investigated the use of parallel methods of optimization for use in the optimal management formulation. These included an evolutionary computing method called genetic optimization and a modified version of the direct search method of optimization called the Shuffled Box Complex method of constrained optimization. The resulting optimal management model obtained by linking macro-level simulation models with efficient optimization models is capable of identifying optimal management strategies for an urban watershed to satisfy water

quality and economic related objectives. Finally, the optimal management model is applied to a real world urban watershed to evaluate management strategies for water quality management leading to the selection of near-optimal strategies.

KEYWORDS: Evolutionary Algorithms, Optimization, Macro-level Simulation Models, Water Quality, Watershed management

Mohammad Tufail

May 4, 2006

OPTIMAL WATER QUALITY MANAGEMENT STRATEGIES FOR URBAN WATERSHEDS USING MACRO-LEVEL SIMULATION MODELS LINKED WITH EVOLUTIONARY ALGORITHMS

By

Mohammad Tufail

Dr. Lindell E. Ormsbee

Director of Dissertation

Dr. Kamyar C. Mahboub

Director of Graduate Studies

Date: May 4, 2006

DISSERTATION

Mohammad Tufail

The Graduate School

University of Kentucky

2006

OPTIMAL WATER QUALITY MANAGEMENT STRATEGIES FOR URBAN WATERSHEDS USING MACRO-LEVEL SIMULATION MODELS LINKED WITH EVOLUTIONARY ALGORITHMS

DISSERTATION

A dissertation submitted in partial fulfillment of the requirements
for the degree of Doctor of Philosophy in Civil Engineering at the
University of Kentucky

By

Mohammad Tufail

Lexington, Kentucky

Director: Dr. Lindell E. Ormsbee, Professor of Civil Engineering

Lexington, Kentucky

2006

ACKNOWLEDGMENTS

This research was funded by a grant from the Kentucky Division of Water under Grant No. 200304300958. The work was completed at the Kentucky Water Resources Research Institute at University of Kentucky under the direction of Dr. Lindell E. Ormsbee, Professor of Civil Engineering at the University of Kentucky. The author is grateful to the Institute and the Department of Civil Engineering for the financial support extended to him during the research.

The author feels an enormous debt of respectful gratitude to his major advisor, Dr. Lindell Ormsbee, for his valuable and thoughtful guidance, keen interest, and constant encouragement throughout the course of this research effort. In particular, the author is grateful to Dr. Ormsbee in training him to think critically, innovatively, and outside the box to seek solutions to problems encountered at various stages of this research. The author would also like to thank his remaining members of the doctoral committee for their help and suggestions during the research work. In particular, the author would like thank Dr. Srinivasa Lingireddy for his guidance and encouragement.

The author is also grateful to two visiting research scholars at the University of Kentucky (Dr. Ramesh Teegavarapu and Dr. V. Chandramouli) for their guidance and support throughout this research. The author wishes to extend thanks to the staff of Metropolitan Sewer District (MSD) Louisville, Kentucky for their assistance in supplying the data collected in support of the Beargrass Creek watershed TMDL project. The author is also thankful to Lynn Jarrett of JE Edinger Associates, Inc. for providing useful information about the dissolved oxygen dynamics in Beargrass Creek watershed, Louisville, Kentucky.

The author is indebted to his parents, Mr. Gul Afzal Khan and Mrs. Tajbar Sultan, for their affection and prayers throughout the course of this work. Author also wishes to thank his siblings and all other family members for their affection and support. Special thanks are due to the author's wife (Uzma) and daughters (Maryam and Zaynab), who's patience, understanding, and love has been the source of encouragement to him. The author would also like to thank all his friends who supported him during this research. In particular, the author would like to thank fellow PhD candidate, Pani Ramalingam, for his friendship, support and help throughout the course of this work.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER 1
INTRODUCTION

1.1 Problem Statement

According to the 2000 National Water Quality Inventory report, about 40% of the assessed streams in the U.S. were not clean enough to support designated uses such as fishing and swimming. Leading causes of impairment in these assessed waters include bacteria, nutrients, metals (primarily mercury), and siltation. Runoff from agricultural lands, municipal point sources (sewage treatment plants and combined sewer overflows), and hydrologic modifications (such as channelization, flow regulation, and dredging) are the primary sources of impairment. Although the United States has made significant progress in cleaning up polluted waters over the past 30 years, much remains to be done to restore and protect the nation's waters (EPA, 2002). In the United States, many federal and state level environmental policies and regulations have been initiated to control such problems. These include policies and programs such as the Clean Water Act (CWA) (Federal Register, 1972), the Federal TMDL (Total Maximum Daily Load) program (Federal Register, 1972), and programs for the control and management of combined sewer overflows (CSOs) and sanitary sewer overflows (SSOs). The TMDL regulations that currently apply are those that were issued in 1985 and amended in 1992 (40 CFR Part 130, section 130.7).

Both point and non-point sources of pollution are internationally recognized as critical environmental problems. In recent years it has become increasingly obvious to EPA that in order to enhance and achieve the objectives of the Clean Water Act, an *integrated watershed management approach* is needed that addresses both *point* and *non-point* s*ources* of pollution affecting a watershed.

Watershed management is a complex process that involves multiple uses and diverse stakeholders (Dorn, 2004). Complex watershed management requires the use of a variety of computer-based hydrologic, hydraulic, and water quality models. These simulation models are used to quantify the impact of hydrologic and water quality processes

occurring in a watershed. The use of accurate and practical simulation models plays an important role in watershed management. Such models can be used to identify effective management solutions to restore water quality in watersheds. The goal in most cases is to select a strategy (solution) that meets all economic, environmental, and other objectives. In cases where multiple feasible scenarios need evaluation, the use of simulation models alone can be cumbersome, time consuming, and cost prohibitive. In such situations, an optimization model coupled with simulation model(s) can be used to identify optimal solutions. Such a comprehensive approach of watershed management is an emerging science (Muleta, 2003) and there is a need to develop more efficient and practical tools to assist in such an approach.

Urban watershed management poses a very challenging problem due to the various sources of pollution and there is a need to develop optimal management models that can facilitate the process of identifying optimal management strategies. An optimal management formulation for urban watersheds should consist of effective and practical simulation model structures as well as efficient optimization algorithms. For such an optimal management formulation to be effective, it should allow the evaluation of management strategies that address both point and non-point sources of pollution. Finally, the optimal management formulation should result in alternatives that are feasible as well as practical and meet both water quality as well as economic objectives.

It is increasingly evident that most water quality problems in urban watersheds are complex and require costly solutions. There continue to be a need for management tools and methodologies that can guide decision makers in formulating solutions to such complex problems that are both least-cost and environmentally sustainable. By necessity, such tools will require a linkage of water quality simulation models with optimization models in an effective and efficient manner. Since most existing comprehensive water quality simulation models do not lend themselves for integration into such an environment, there is a need to develop simpler models to represent the response of hydrologic and water quality processes in such watersheds. Such macro-level models can be more effectively linked with efficient optimization models to provide a decision

support system for watershed managers. The need for macro-level models was recently highlighted in the National Research Council (NRC, 2001) report that assessed the scientific basis of the Federal TMDL Program (40 CFR Part 130, section 130.7). The NRC report recommended that "Given the variety of existing watershed and water quality models available, and the range of relevant model selection criteria, EPA should expand its focus beyond mechanistic process models to include simpler models (NRC, 2001)." In the same context, the report also recommended that "EPA should support research in the development of simpler mechanistic models that can be fully parameterized from the available data (NRC, 2001)."

1.2 Summary of Previous Work

Due to the fact that comprehensive watershed management is an emerging and rather challenging area for researchers, there are relatively few applications that exist (Muleta, 2003). Ormsbee (1983) lists some of the contributions in the area of urban watershed management, particularly in studying the problem of optimal placement of detention basins in an urban watershed. These include Abt and Grigg (1978), Mays and Bedient (1982), and Flores et al. (1982). Ormsbee (1983) presented a methodology for use in the planning of dual purpose detention basins in urban watersheds. The methodology employed continuous simulation, statistical analysis, and a design heuristic to obtain an integrated system of detention basins. The methodology was capable of handling both water quantity and quality considerations.

Recently, Muleta (2003) summarized a list of contributions in the area of watershed management. These include contributions by Harrell and Ranjithan (1997), Sengupta (2000), Dorn et al. (2001), Zhen and Yu (2002), and Srivastava et al. (2002). More recent contributions include those of Zechman (2005) and Dorn (2004). Muleta (2003) developed an integrative computational methodology for the management of non-point source pollution from agricultural watersheds. The method is based on an interface between evolutionary algorithms (EAs) and a comprehensive watershed simulation model known as Soil and Water Assessment Tool (SWAT).

Dorn (2004) developed a new evolutionary algorithm based technique for systematic generation of alternatives and multi-objective optimization to aid in watershed management. The new EA-based framework focused on storm water management issues such as use of best management practices (BMPs) to control runoff resulting from new developments. In particular, the modeling and management framework was applied to watersheds for obtaining cost-effective system of pipes and dry detention ponds to convey runoff generated by a design storm while meeting objectives of runoff control. The optimization model developed in the study is linked with a storm water simulation model (called SWMM – Storm Water Management Model) developed by EPA.

Zechman (2005) developed a new model error correction procedure to improve the predictive capabilities of simulation models for use in watershed management. The work also results in new evolutionary computation (EC) based methods to generate alternatives for numeric and symbolic search problems. The alternatives generation procedure developed are then coupled with the model error correction procedure to improve predictive capabilities of simulation models and to address the non-uniqueness issue.

1.3 Research Needs

Based on a review of the most recent research in the area of optimal watershed management, several research needs were identified. These are listed as follows:

1. There continues to exist a need for an *optimal management framework* for urban watershed management that addresses both point and non-point pollution sources.
2. There continues to exist a need for *efficient macro-level* water quality simulation models for use in such a framework.
3. There continues to exist a need for *efficient nonlinear constrained optimization models* for use in such an optimal management framework.

1.4 Research Questions

This dissertation will investigate the following four research questions as they relate to water quality modeling and management of urban watersheds that are impaired due to point and non-point sources of pollution:

1. Can macro-level (simplified) models be used in lieu of more complex deductive model(s) in providing a sufficient cause and effect relationship on which to base sound management decisions?
2. Can macro-level models be effectively integrated into a nonlinear constrained optimization framework so as to provide an effective decision-making tool for evaluating optimal water quality strategies for watershed management?
3. What types of macro-level simulation models are most efficient in generating such optimal management strategies?
4. What types of optimization models are most efficient in generating such optimal management strategies?

1.5 Research Objectives

The objective of this research is to develop a screening level, comprehensive and integrated computational methodology that can be used by decision makers to evaluate cost-effective water quality management strategies leading to reduction of point and non-point source pollution in urban watersheds. The research will investigate the utility of macro-level water quality simulation models for use in an integrated watershed management framework. An optimal management model will thus be developed by linking a macro-level water quality model with an efficient optimization model (Figure 1-1).

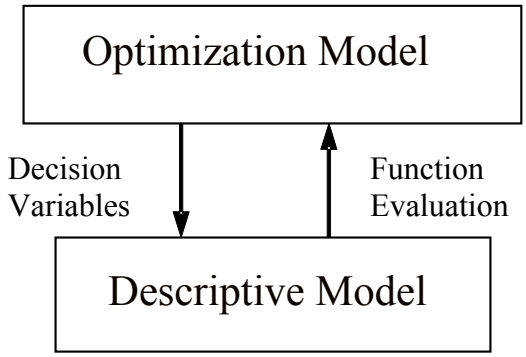


Figure 1-1. Proposed Framework of the Optimal Management Model

This is a disaggregated approach of formulating an optimal management problem in which a set of decision variables are passed on from the optimization model to the simulation model. The simulation model evaluates the system equations and any constraints that are being considered, and returns the information back to the optimization model. Based on the information passed to the optimization model, a particular solution set or strategy is assigned an objective function value or fitness value. The process continues and different solution sets are evaluated and ranked based on their fitness value leading to the selection of the optimal solution set or strategy. Thus there are two distinct components of the optimal management model namely 1) the water quality simulation model, and 2) the optimization model. This research will investigate the utility of macro-level water quality simulation models in lieu of the traditional and complex process-based (deductive) models in developing optimal load reduction strategies for complex urban watersheds affected by both point and non-point source pollution.

The systematic analysis of a complex urban watershed will frequently require the application of multiple deductive models of watershed processes. While such deductive models can be expected to better reflect the true dynamics of the process or processes being modeled, such models may not be ideally suited for application in an integrated watershed management framework. In many cases, the linkage of such deductive models with an associated optimization model may not be feasible or even physically possible. In such an environment, more compact and computationally efficient macro-level models

may be necessary. If macro-level models can be shown to produce comparable management decisions to those solutions obtained using more comprehensive deductive models, then the use of such efficient macro-level models can be justified. In theory, three different levels or types of macro-level simulation models are possible namely 1) implicit inductive models, 2) explicit inductive models, and 3) simplified deductive models. This research will investigate the utility of the last two classes of models (explicit inductive and simplified deductive) in the context of an optimal watershed management framework. State-of-the-art operations research techniques will be explored for use in developing the explicit inductive models. In particular, these techniques range from simple regression models to more complex and nonlinear models such as artificial neural networks (ANNs). A genetic algorithm-based function approximation technique recently developed by the author named FFSGA (Fixed Functional Set Genetic Algorithm) approach will also be investigated for use in developing macro-level models.

In the context of optimization methods, the research will investigate the utility of linking macro-level simulation models with "parallel" methods of optimization. Specifically, the utility of two different types of optimization techniques will be investigated for use in the proposed optimal management model. These include 1) an evolutionary computation-based method called genetic optimization (Goldberg, 1989) and 2) a modified version of the direct search method of optimization called the Box Complex method of constrained optimization (Box, 1965). This modified method is named Shuffled Box Complex method of constrained optimization. Finally, the research will evaluate the utility of the proposed optimal management model in application to a real world problem. The proposed methodology uses practical and state-of-the-art knowledge from different interconnected disciplines of hydrology, operations research, artificial intelligence, and watershed management. The research objectives are in line with the short and long-term goals of the CWA (Federal Register, 1972), the Federal TMDL Program (40 CFR Part 130, section 130.7), and recommendations of the NRC report (NRC, 2001).

1.6 Research Application

The modeling methodology developed in this dissertation will be used to address the environmental problems of the Beargrass Creek watershed in Jefferson County, Louisville, Kentucky (Figure 1-2). The watershed contains three different sub-basins all of which have been placed on the State of Kentucky's 303(d) List of Impaired Water Bodies since the early 1990's for pathogens and dissolved oxygen/organic enrichment. The sources of pollution include storm water runoff as well as wet weather discharge from numerous CSOs and SSOs.

The Louisville and Jefferson County Metropolitan Sewer District (MSD) provides sanitary sewer, storm water drainage, and flood protection services for all of Jefferson County. The Commonwealth of Kentucky filed a civil suit against MSD in state court in February, 2004 for unlawful discharge of untreated sewage and overflows of combined sewage into the Ohio River and its tributaries totaling billions of gallons each year. The U.S. Department of Justice, U.S. Environmental Protection Agency, and Commonwealth of Kentucky's Environmental and Public Protection Cabinet (EPPC) jointly signed a consent decree on April 25, 2005 for a comprehensive Clean Water Act settlement with the Louisville and Jefferson County Metropolitan Sewer District (MSD). The settlement requires that MSD will make extensive improvements to its sewer systems to eliminate unauthorized discharges of untreated sewage and to address problems of overflows from sewers that carry a combination of untreated sewage and storm water at a cost likely to exceed $500 million (U.S. Department of Justice, 2005).

To restore these water bodies to compliance, the Louisville and Jefferson County MSD is in the process of establishing Total Maximum Daily Loads (TMDLs) for each of the three sub-basins of the Beargrass Creek watershed as well as developing a long term control plan (LTCP) that will enable them to achieve such loads. In support of the development of the pathogen and nutrient TMDL for these sub-basins, a comprehensive water quality monitoring and modeling effort is underway. Data for this watershed will be used in the development of macro-level water quality models and optimal management models for

the Beargrass Creek watershed. Beargrass Creek is an urban and complex watershed that is impaired due to both point and non-point sources of pollution and thus provides an excellent opportunity to evaluate the utility of the proposed methodology.

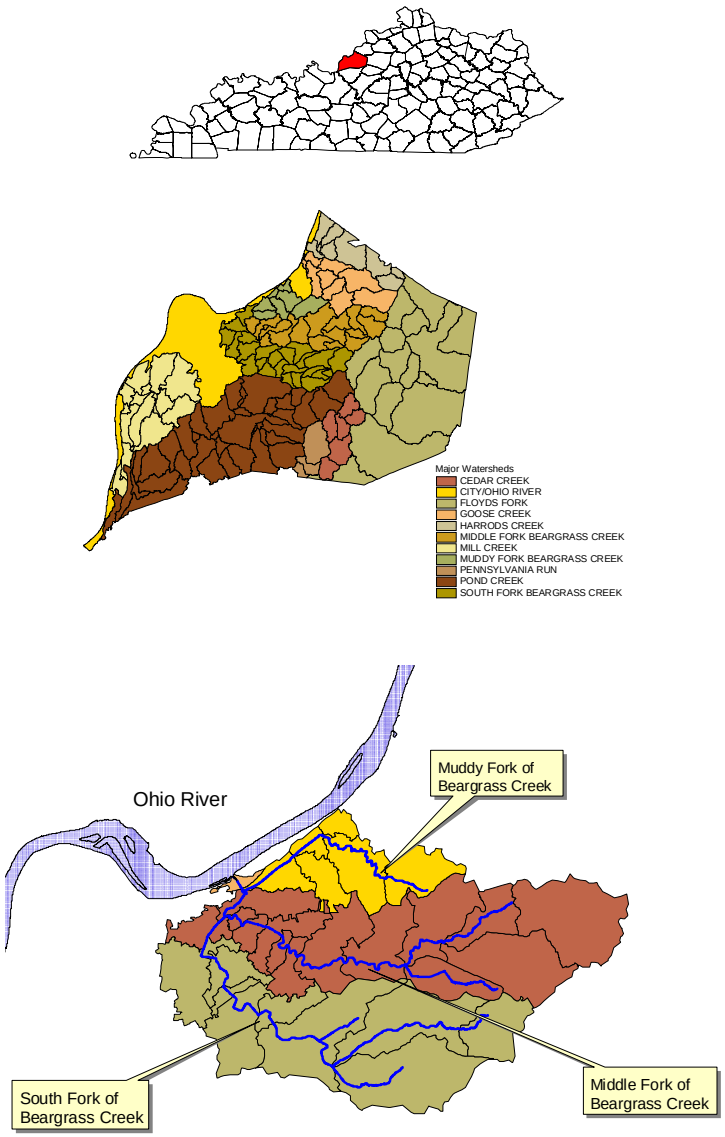


Figure 1-2. Beargrass Creek Watershed, Louisville, Jefferson County, Kentucky

The proposed optimal management model will be used as a screening tool to evaluate least cost water quality management strategies for the Beargrass Creek watershed that is impaired by multiple sources (i.e. CSOs, leaking sewers, and non-point source pollution). Alternatively, the optimal management model will also be used to develop water quality management strategies as constrained by a specified budget.

1.7 Significant Contributions of the Research

The unique contributions of this research are summarized as follows:

1. A comprehensive and screening level optimal management model for integrated watershed management is developed for complex urban watersheds impaired by both point and non-point sources. The management model is obtained by linking macro-level water quality simulation models with efficient optimization models in a disaggregated constrained optimization framework. The proposed framework makes use of a novel inverse loading deductive model for simulating dissolved oxygen linked with a new, highly efficient optimization method called the Shuffled Box Complex method.
2. A macro-level approach of water quality simulation modeling is proposed for use in an optimal management framework. Such an approach provides greater flexibility and allows for the use of several different types of simulation model structures for use in the optimal management model and results in significant savings in computational time when compared to more traditional process-based simulation models.
3. A novel simple deductive model is developed to simulate the dissolved oxygen (DO) and biochemical oxygen demand (BOD) dynamics in an urban watershed impaired by wet weather flows from CSO discharges, urban runoff, and leaking sewers along stream banks. This inverse loading model is based on the classic Streeter-Phelps equation (Streeter and Phelps, 1925) for modeling dissolved oxygen deficit in a water column and is calibrated using observed dissolved oxygen data collected in the watershed to back-calculate the corresponding effective BOD concentration that is causing the DO deficit in the stream reach. The effective BOD loads (concentration

and flows) are then disaggregated into different components corresponding to the source of pollution (i.e. point, non-point, and other). Once the BOD loads are disaggregated, the model is run in the forward direction to simulate DO response in the watershed. An added advantage of this inverse load model is that it eliminates the use of a rainfall-runoff model (and thus the error associated with it) by using observed stream flows in the simple deductive model.

4. A new genetic algorithm-based technique for inductive model construction is developed called FFSGA (fixed functional set genetic algorithm). FFSGA can be effectively used to develop inductive (empirical) models for a response function in the area of water resources and environmental engineering and management. This new technique competes well with existing state-of-the-art techniques used for inductive model development such as artificial neural networks (ANNs) and genetic programming (GP) (Tufail and Ormsbee, 2004; Tufail and Ormsbee, 2006). An added advantage of FFSGA over other state-of-the-art techniques such as ANNs and GP is that it results in a compact, simple, and easy to use expression for a response function modeled.
5. This research investigated the use of two different types of optimization techniques (genetic algorithms and Shuffled Box Complex method) for use in the optimal management model to evaluate their relative performance and applicability to watershed management problems. The Shuffled Box Complex method of constrained optimization is a new method that is based on the original Box Complex method of constrained optimization (Box, 1965). The new method introduces the concept of multiple complexes and random shuffling in the original Box Complex method and application results demonstrates that the modified Shuffled Box Complex method can be successfully applied to watershed management problems with performance superior or equal to that of genetic algorithms. The advantage of using Shuffled Box Complex over genetic algorithms (GAs) is that it is relatively simple and it eliminates the use of penalty functions to handle inequality constraints in the optimal management model. The use of penalty functions in using GAs for constrained optimization can be considered as a drawback as they can require extensive fine tuning and parameter estimation.

1.8 Organization of the Dissertation

This dissertation is organized into eight chapters as follows. Chapter 1 provides an introduction to the research that consists of a problem statement, summary of previous work, research needs, research questions, research objectives, research application, and significant findings of the research. Chapter 2 presents a discussion on optimization methods that can used in an optimal management framework. In particular, two types of optimization techniques are discussed in detail namely an evolutionary-based method called genetic algorithms (GAs), and a direct search method called Shuffled Box Complex method of constrained optimization. Chapter 3 presents a literature review of mathematical models for watershed management. A review of both deductive and inductive models and their methods of analysis are presented in this chapter. Chapter 4 presents a new approach for function approximation called Fixed Functional Set Genetic Algorithm (FFSGA). FFSGA can be effectively used to develop inductive and macro-level simulation models for a response function in water resources engineering and management. Chapter 5 is devoted to the development of a series of macro-level water quality simulation models. These include 1) explicit inductive models for pathogens, nutrients, and dissolved oxygen response in a watershed, and 2) a simplified deductive and inverse loading model for dissolved oxygen response in an urban watershed. Chapter 6 presents the mathematical formulation of the proposed optimal management model. Chapter 7 presents the application of the optimal management model to a real world watershed that is impaired by point and non-point sources of pollution. The watershed used for this application is the Beargrass Creek watershed in Louisville, Kentucky. Finally, the conclusions and recommendations of the research are summarized in Chapter 8.

CHAPTER 2
OPTIMIZATION FOR WATERSHED MANAGEMENT

2.1 Introduction

A common problem encountered by engineers in all fields is the problem of finding an optimal policy for a system under study. Optimization is often applied to solve such problems in order to maximize the benefits and minimize the associated costs. The theory of optimization finds applications in all branches of engineering at different levels. Some example areas of application include design, planning and analysis of existing systems, and control of dynamic systems (Reklaitis et al. 1983). In most engineering applications, optimization is linked to a mathematical model of the system that is used to analyze and characterize the performance of the system.

Watershed simulation models are frequently used to predict hydrologic and water quality responses for a variety of applications such as real time control of separate and combined sewer systems, impacts of combined sewer overflows and urban runoff on receiving waters, and evaluation of different management strategies for watershed pollution control. Broadly speaking, the use of simulation models can fall into one or both of two major categories namely, 1) for use as an analysis or evaluation tool for engineers and scientists and 2) for use as design or management tool for decision makers. In the latter case, the use of simulation models alone may not be the best way to achieve management objectives in which multiple strategies are evaluated to obtain the optimal solutions. The number of design or management scenarios that may exist can be so large that a manual or trial and error investigation of such scenarios using simulation models alone can be cumbersome and tedious (Muleta, 2003). In such applications, there is a need for an integrated management approach that uses an optimization technique linked to a simulation model to achieve optimal solutions. Such an approach will allow the decision makers to choose the best solution that satisfies all constraints by evaluating multiple feasible management strategies in an effective manner.

In the context of watershed management, an optimal management formulation can be very useful to help watershed managers evaluate optimal management strategies needed to achieve water quantity and quality objectives. Such a formulation will consist of an optimization model linked to one or more set of watershed models that simulates hydrologic and water quality processes and their impacts on the receiving waters in the watershed and is schematically shown in Figure 2-1 below.

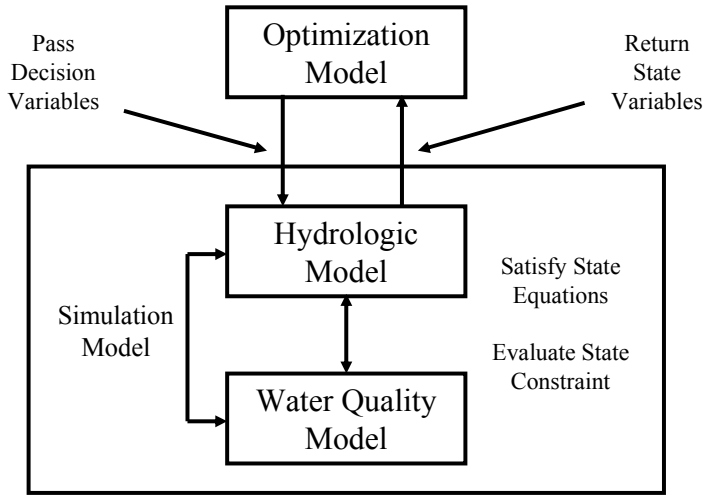


Figure 2-1. Optimization Formulation for Watershed Management

The choice of optimization technique to be linked with a simulation model for watershed management depends on the particular application and its complexity. Traditional optimization methods (e.g. simplex method, steepest descent method) are known to perform well for mostly linear or quadratic functions. Hydrologic and water quality processes occurring in a watershed are known to be highly non-linear and complex and the use of traditional optimization techniques are limited for such applications. In such applications, traditional methods typically lack robustness and require continuous search spaces with defined derivatives. Even when the processes are simplified and linearized, such techniques are known to produce questionable results in their application to multi-modal functions (Muleta, 2003). The use of evolutionary methods for complex processes tends to overcome some of the shortcomings of the traditional methods. Evolutionary methods can handle large search spaces, do not require derivatives of the functions,

performs simultaneous evaluation of multiple solution vectors, and are particularly suited for large non-convex problems. These advantages make them a suitable choice for use in conjunction with a water quality simulation model for watershed management, which is one of the objectives of this study. In this research, the utility of two types of optimization models linked to macro-level simulation models are investigated in solving the optimal watershed management problem due to point and non-point sources of pollution.

2.2 Definition of the Optimal Management Problem

Optimization problems are mathematically formulated to include an objective function that is optimized (maximized or minimized) subject to a set of constraints, which can be a set of algebraic equations and/or inequalities. The set of algebraic equations can be represented by a simulation model of the particular system being modeled. Such a mathematical formulation or framework leads to the development of an *optimal management model* which can be used in the optimal design and operation of the system. More specifically, the optimal management problem can be stated as follows (Mays, 1997):

Given:

1. The state equations
2. A set of boundary conditions on the state variables at the initial time and the terminal time
3. A set of constraints on the state variables and the control variables

Determine the optimal (and admissible) values of the control variables so that a performance index (an objective function) is optimized (minimized or maximized).

In its most general form, the optimal management problem may be formulated as non-linear optimization problem given as follows (Equations 2-1 to 2-4):

Minimize or Maximize:	$\mathbf{F(X)}$	(2-1)
Subject to:	$\mathbf{g(X) = 0}$	(2-2)
	$\mathbf{h(X) > 0}$	(2-3)
	$\mathbf{X_{min} < X < X_{max}}$	(2-4)

Where X represents a vector of decision variables, F(X) represents the objective function to be maximized or minimized, g(X) represents the explicit or implicit system constraints to be satisfied, and h(X) represents the implicit bound constraints to be satisfied by the optimal management formulation. X_{min} and X_{max} represent the explicit bound constraints on the decision variables of the optimal management formulation. The system constraints can be represented explicitly by the use of a set of linear or nonlinear equations or implicitly by the use of a simulation model (Ormsbee and Reddy, 1995). When using an implicit formulation, the system equations can be represented using either an inductive or deductive formulation.

2.3 Types of Approaches in an Optimal Management Problem

In most applications, the optimal management problem can be formulated in one or two distinct ways. These include 1) a composite approach, where the explicit system constraints are lumped and solved with the corresponding bound constraints (e.g. the traditional linear programming formulation) or 2) a disaggregated approach, where the system constraints are separated from the optimization problem and explicitly enforced through simulation. These are shown in Figures 2-2 and 2-3 below.

Optimization Model

MIN: F(X)

ST: g(X) = 0
h(X) > 0
$X_{min} < X < X_{max}$

Figure 2-2. Composite Optimization Framework

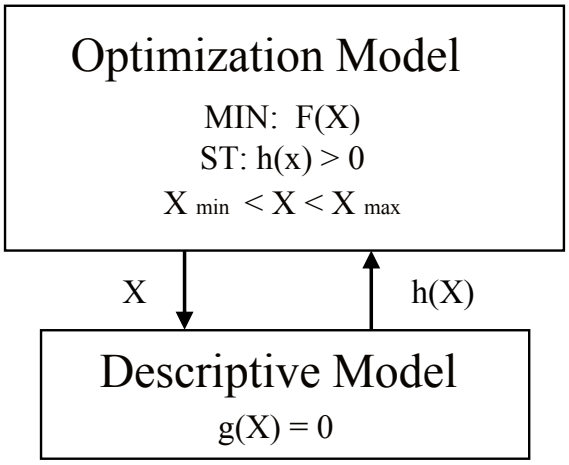


Figure 2-3. Disaggregated Optimization Framework

This research is focused on the application of the disaggregated approach to optimal management of water quality in urban watersheds. Such an optimal management formulation is comprised of two distinct components namely 1) an optimization model and 2) a descriptive model of the system or process for which the optimal management model is sought (Tufail and Ormsbee, 2005a).

The disaggregated approach was chosen due to its flexibility in allowing the effective evaluation of different model structures for both optimization and descriptive models. Contrary to the composite approach, the mathematical programming in the disaggregated approach is less complex and easier to implement. The next two sub-sections will describe some of the available choices for descriptive models as well as optimization algorithms for use in the disaggregated approach of optimal management formulation given in Figure 2-3.

2.3.1 Types of Descriptive Models in an Optimal Management Problem

A descriptive model can be represented in different ways in an optimization framework and Figure 2-4 and Table 2-1 below gives the broad classes of models that can be used to represent a descriptive model of a system.

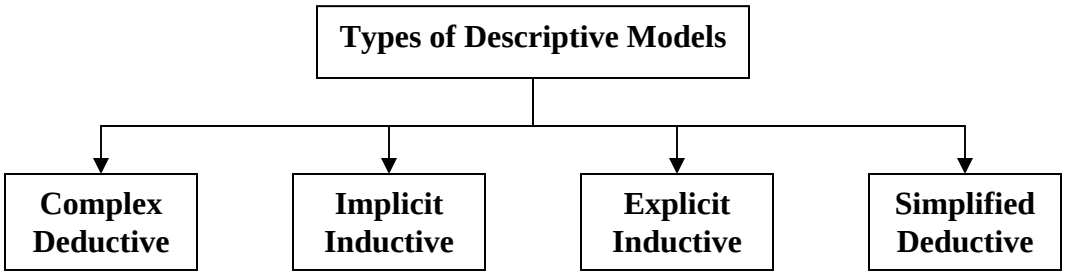


Figure 2-4. Classes of Descriptive Models used in Optimal Management Problems

Table 2-1. Examples of Descriptive Model Classes

Descriptive model approaches	Example model or method
Complex deductive model	HSPF/SWMM/WASP/CEQUAL-RIV1
Explicit inductive model	Regression/Neural Networks models using raw data
Implicit inductive model	Regression/Neural Networks using output from a calibrated deductive model
Simplified deductive model	Streeter-Phelps inverse load model

2.3.1.1 Complex Deductive Model

This approach requires the use of a complex deductive model linked to an optimization algorithm (per the framework given in Figure 2-3). This approach can be computationally very expensive since most complex deductive models require significant time, particularly if applied to perform a continuous simulation over a longer period of time. The transfer of control variables between the simulation model and optimization algorithm can thus be very time consuming. For these reasons, this approach may not be very favorable for scenarios where multiple management scenarios need to be evaluated in a short period of time. In addition, for more complex applications involving multiple deductive models, it may not be practical or even physically possible to embed the simulation models with an optimal management framework.

2.3.1.2 Implicit Inductive Model

An implicit inductive model is constructed by utilizing output data from a calibrated deductive model of the process or system being modeled. This approach can be useful in

situations where 1) a fully calibrated deductive model is available but it is very complex for integration into an optimization framework and thereby computationally expense, and 2) there is lack of raw data needed to develop an explicit inductive model. Implicit inductive models can result in significant computational savings and may be more favorable if quick decisions are needed over a short period of time. A certain degree of caution needs to be exercised in the development of implicit inductive models for integration into an optimization framework. Such a caution means that the resulting implicit models should capture the dynamics of the process with acceptable confidence in order to serve as a substitute for the calibrated deductive model. This can be verified by comparing the performance of the implicit inductive model versus the calibrated deductive model using the same set of independent variables.

2.3.1.3 Explicit Inductive Model

An explicit inductive model can be constructed when sufficient data are available to permit the development of an inductive relationship between the independent and dependent variables. Such models may be developed using various techniques such as linear or nonlinear regression, artificial neural networks (ANNs), or other evolutionary methods such as genetic programming and genetic functions. The development of explicit inductive models requires sufficient raw data over a range of time to fully capture the behavior of the response function being modeled. The use of explicit inductive models in an optimization framework can be a favorable choice due to their ease of use and simplicity as substitutes for more process-based deductive models. For instance, explicit inductive models may be preferred where 1) computational expense is a critical issue, 2) the process-based deductive model is over parameterized and cannot be adequately calibrated, and 3) budgetary constraints do not allow for a complex deductive model. While such an approach can result in significant computational savings resulting in an efficient and effective optimal management framework, it is important to make sure that the resulting model is capable of accurately representing the response function. This can be verified by evaluating the assumed cause and effect relationship between input and output variables through the process of model validation.

2.3.1.4 Simplified Deductive Model

A simplified deductive model can be constructed for a particular response function for integration into an optimization framework when either of the following scenarios is valid:

- A comprehensive calibrated deductive model is not available due to reasons such as budgetary constraints.
- A comprehensive calibrated deductive model requires excessive computation time.
- The deductive model consists of multiple complex deductive models which make it too complex to allow effective integration into the optimization framework.
- An explicit inductive model is not available due to data scarcity.
- An explicit inductive model does not fully capture the dynamics of the response function being modeled, that is it fails to accurately validate the cause-and-effect relationship between input and output variables.
- An implicit inductive model is not available due to unavailability of a calibrated deductive model.
- An implicit inductive model does not capture the full dynamics of the response function as modeled in the calibrated deductive model.

In this approach, a model of the system response function can be constructed by using a simplified approach to modeling. Thus rather than constructing a comprehensive dynamic model for a system, one or more simplified model representations of the process or processes are constructed. This is achieved by making reasonable assumptions about the system and validating the resulting models using any available data sets. For example, under the appropriate conditions, the Kinematic Wave model may serve as a reasonable approximation of the St. Venant Equations for fully dynamic flow in an open channel. Alternatively, the Streeter-Phelps model (applied over daily time step for simulating dissolved oxygen in a stream) may serve as a reasonable substitute for a more complex deductive water quality model for simulating dissolved oxygen such as HSPF or WASP or CE-QUAL2-RV1. Such an approach has the advantage of reducing

computational time when integrated into an optimization framework and can provide an effective planning tool for evaluating multiple screening level management alternatives in the optimal management problem.

2.3.2 Types of Optimization Models in an Optimal Management Problem

Various optimization algorithms have been developed for solving different optimization problems. In general, optimization algorithms may be subdivided into two broad classifications: constrained optimization methods and unconstrained optimization methods. Unconstrained methods are for use in solving Equation (2-1) only, while constrained methods are for use in solving problems involving Equations (2-1) to (2-4). Constrained methods can further be subdivided into linear problems or nonlinear problems. Due to the constrained nature of the watershed management problem, only those methods applicable to nonlinear constrained problems will be examined.

Nonlinear constrained methods can broadly be classified into four categories namely 1) exhaustive search or optimal enumeration methods, 2) gradient-based methods, 3) direct search methods, and 4) evolutionary methods as shown in Figure 2-5 and Table 2-2. The choice of a particular method depends on many factors such as the functional form of the objective function and the associated constraints, user preference, knowledge of technique, complexity of the application and other application-specific needs.

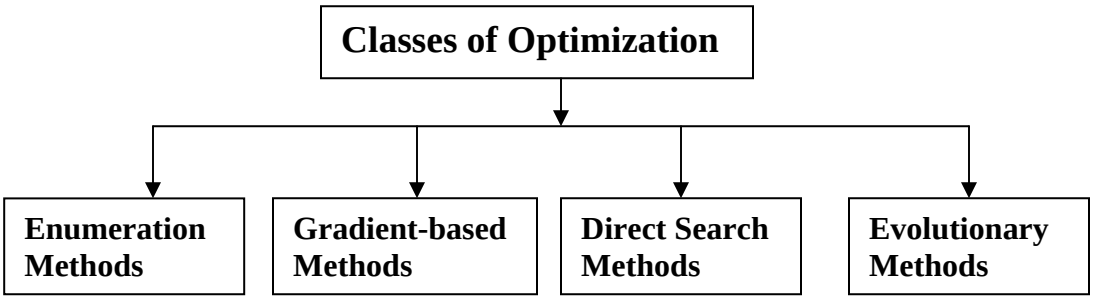


Figure 2-5. Classes of Optimization Techniques

Table 2-2 Examples of Optimization Classes

Class of Optimization methods	Example method
Optimal enumeration methods	Dynamic Programming
Gradient-based methods	Generally Reduced Gradient (GRG)
Direct search methods	Box Complex
Evolutionary computing methods	Genetic Algorithms

2.3.2.1 Optimal Enumeration Methods

In optimal enumeration methods, the search algorithm evaluates the objective function value at each point in the feasible search space. An example of this optimization method is the traditional Dynamic Programming (DP). While very efficient for a particular subset of constrained nonlinear problems, DP is largely restricted to problems that can be separated into a series of independent problems or to those that involve only a small number of decision variables (Bellman, 1961). Unfortunately, the watershed management problem under consideration does not satisfy these restrictions.

2.3.2.2 Gradient-based Methods

Gradient based methods seek to minimize an expanded objective function made up of the original objective function (i.e. Equation 2-1) and a penalty term that incorporates the degree of violation of the associated constraints (i.e. Equations 2-2 through 2-3). The expanded formulation is minimized by seeking to determine the values of the decision variables in the objective function that will yield a function gradient equal to zero. The primary limitations of the method are due to 1) the requirement for gradients or higher order derivatives of the composite objective function, 2) the need for an iterative process to fine tune the weights associated with the penalty term in order to avoid a numerical distortion of the solution space, and 3) the potential convergence of the method to a sub-optimal solution in those problems that may possess many alternative optimal solutions. Each of the three limitations tends to become particularly acute in application to the proposed watershed management formulation. Examples of traditional gradient methods include the steepest descent method (Cauchy, 1847), quasi-Newton methods (Davidon, 1959; Fletcher and Powell, 1963) and conjugate gradient method (Hestenes and Stiefel,

1952). More recently, Abadie and Carpentier (1969) developed a gradient method called the Reduced Gradient method which is able to explicitly handle constraints without the need of a penalty function by breaking the problem into a series of unconstrained problems that are solved using either the conjugate gradient method or the quasi-Newton methods.

2.3.2.3 Direct Search Methods

Direct search methods are similar to gradient based methods in that they seek to yield a search path through the decision space that minimizes the objective function, but dissimilar in that they are able to obtain the incremental search direction without the use of derivatives. Thus they tend to be more applicable to optimization problems formulated using the disaggregated approach. Like gradient methods, constraints are normally handled through the use of a penalty method and thus the method cannot guarantee a global optimal solution due to a directed search along a single search path. Examples of traditional direct search methods include Rosenbrock's algorithm (1960), Powell's method of conjugate direction (Powell, 1964), and the downhill Simplex method of Nelder and Mead (1965). Unlike the methods of Rosenbrock and Powell, the Simplex method is able to search along a single decision path that incorporates a local search around the search direction, thereby increasing the efficiency of the search. One limitation of the Simplex method is that the solution space is investigated along a single search path. However, this limitation has been overcome through the use of multiple simplexes that are used to pursue an optimal solution along multiple simultaneous paths (Duan et al. 1993). Duan et al. (1993) developed a method called Shuffled Complex Evolution (SCE) approach for global minimization in which multiple complexes (simplexes) are evolved in different search paths. In addition to evolving multiple simplexes, the approach by Duan et al. (1993) introduced the idea of shuffling between simplexes in a random manner.

Unlike the previous methods which were applied only to unconstrained problems, Box (1965) developed a method similar to that of Nelder and Mead (1965) that is applicable

to constrained problems. This was done by explicitly incorporating the constraints into the search space via a constrained simplex which he called a Complex (without the need of a penalty term), thereby greatly improving the efficiency of the overall algorithm. Despite these improvements, the method still suffers from the fact that the solution space is investigated along a single search path, although a more robust one as a result of the use of an expanded complex.

In this research, a new method is proposed called the Shuffled Box Complex method of constrained optimization, which is a modification of the original Box Complex method of constrained optimization (Box, 1965) by introducing the concept of multiple complex evolution and subsequent complex shuffling for constrained optimization problems. The Shuffled Box Complex method was chosen as a candidate for the watershed management problem because 1) the method is conceptually simple, 2) no function derivatives are required, 3) the method is directly applicable to problems involving nonlinear inequality constraints without requiring any transformations and/or use of penalty functions, and 4) the method does not distort the region of search. The next two subsections will describe first the original Box Complex method and then the proposed Shuffled Box Complex method of optimization.

2.3.2.3.1 Box Complex Method

The Complex method of Box (1965) is based on the Simplex method of Spendley, Hext and Himsworth (1962) and has been explained in detail in Ormsbee (1983). The method has successfully been applied to complex nonlinear problems in environmental design (Craig et al, 1978), hydrology (Ormsbee et al. 1984), and water distribution system design (Ormsbee, 1985). It is a direct search technique that moves through the region of search by use of a flexible mathematical figure called a complex. Each vertex in the complex corresponds to a single design. In general, $k \geq (n + 1)$ vertices are used in the complex, where n equals the number of decision variables. Associated with each vertex are n coordinates, with each coordinate corresponding to an individual design variable. The Complex method of Box involves two distinct phases. The first phase involves the

construction of the initial complex. In order to generate an initial complex, an initial vertex corresponding to an initial design must be generated. This initial design must satisfy all constraints (explicit and implicit bound constraints). The remaining (k-1) points needed to set up the initial complex are obtained one at a time by the use of random numbers and bounds for each of the decision variables which are based on the explicit bound constraints for the decision variables as given in Equation (2-4) above. Given upper and lower bounds $X^{(u)}$ and $X^{(l)}$, the pseudo-random variable uniformly distributed on the interval (0, 1) is sampled, and the point coordinates calculated using the following equation.

$$X_i = X^{(l)} + r_i \left(X^{(u)} - X^{(l)}\right) \qquad i = 1, \ldots\ldots N \qquad (2\text{-}5)$$

Where X_i represents the individual design decision variables that make up a solution set, r_i is the random number, and N is the number of points to be generated. A point so selected will satisfy all the explicit bound constraints but not necessarily all the implicit bound constraints. This will require the decision variables to be passed on to the simulation program or any descriptive model that represent the implicit system constraints. If an implicit constraint is violated, then the random point is moved halfway back to the centroid of those points that have already been selected and satisfy all the constraints. Ultimately, a satisfactory point will be found. Following this procedure, the (k-1) additional points can be generated which satisfy all the constraints (Ormsbee, 1986).

The second phase of the Complex method involves the movement of the complex through the solution space. This process is performed using two operations: *complex expansion* and *complex contraction*. These two operations may be visualized as follows. At each stage of movement the objective function is evaluated at each of the points in the complex, and the vertex of the greatest objective function value determined. The complex is then expanded away from this worst point (say P_{high}), through the centroid ($P_{centroid}$) of the remaining points to yield a new point (say P_{new}). Mathematically this may be written as:

$$P_{new} = (1+\alpha)P_{centroid} - \alpha P_{high} \qquad (2\text{-}6)$$

Where α is the expansion coefficient and $P_{centroid}$ is the centroid of all points excluding P_{high}. Box recommended a value of 1.3 for α. The objective function is then evaluated at this new point P_{new}. If the new point yields an objective function value which is better than the worst point P_{high}, then the worst point P_{high} is discarded and the replaced by P_{new}. In this way, the complex moves in the direction of function minimization (see Figure 2-6). If, however, the value of the new point is worse than P_{high}, then the new point is contracted back toward the centroid of the remaining points and a new point $P_{new\text{-}2}$ is generated (see Figure 2-7). This continues until an acceptable point is generated (Ormsbee, 1986). The contraction process can be mathematically represented as follows:

$$P_{new-2} = \omega P_{new} + (1-\omega)P_{centroid} \qquad (2\text{-}7)$$

Where ω is the contraction coefficient for which a value of 0.5 is recommended. This dual process of expansion and contraction continues until some constraint is violated or the algorithm converges. If an independent variable X_i of a new point i violates some explicit bound constraint then that variable is reset to a value just inside the constraint. If the new point violates some implicit bound constraint (inequality constraint) then the point is moved halfway towards the centroid of the remaining points. Eventually a permissible point will be found. The search finally terminates when the complex has collapsed into the centroid (Ormsbee, 1986).

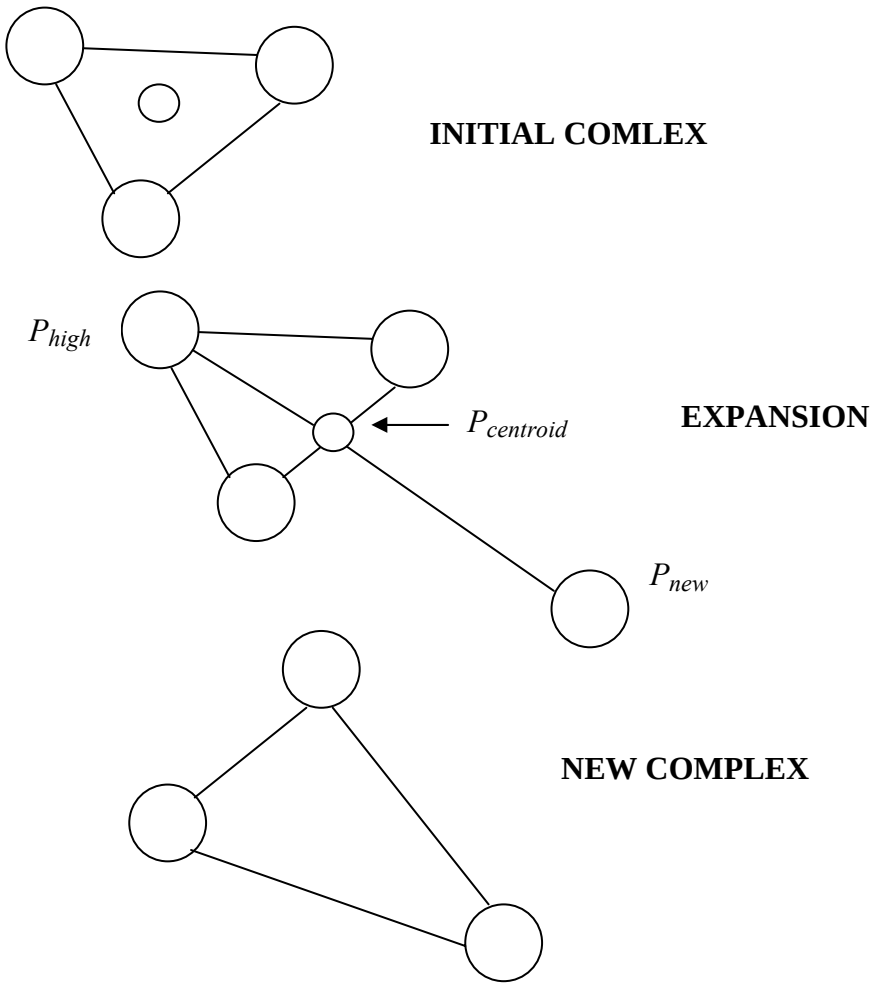


Figure 2-6. Complex Expansion in the Box Complex Method

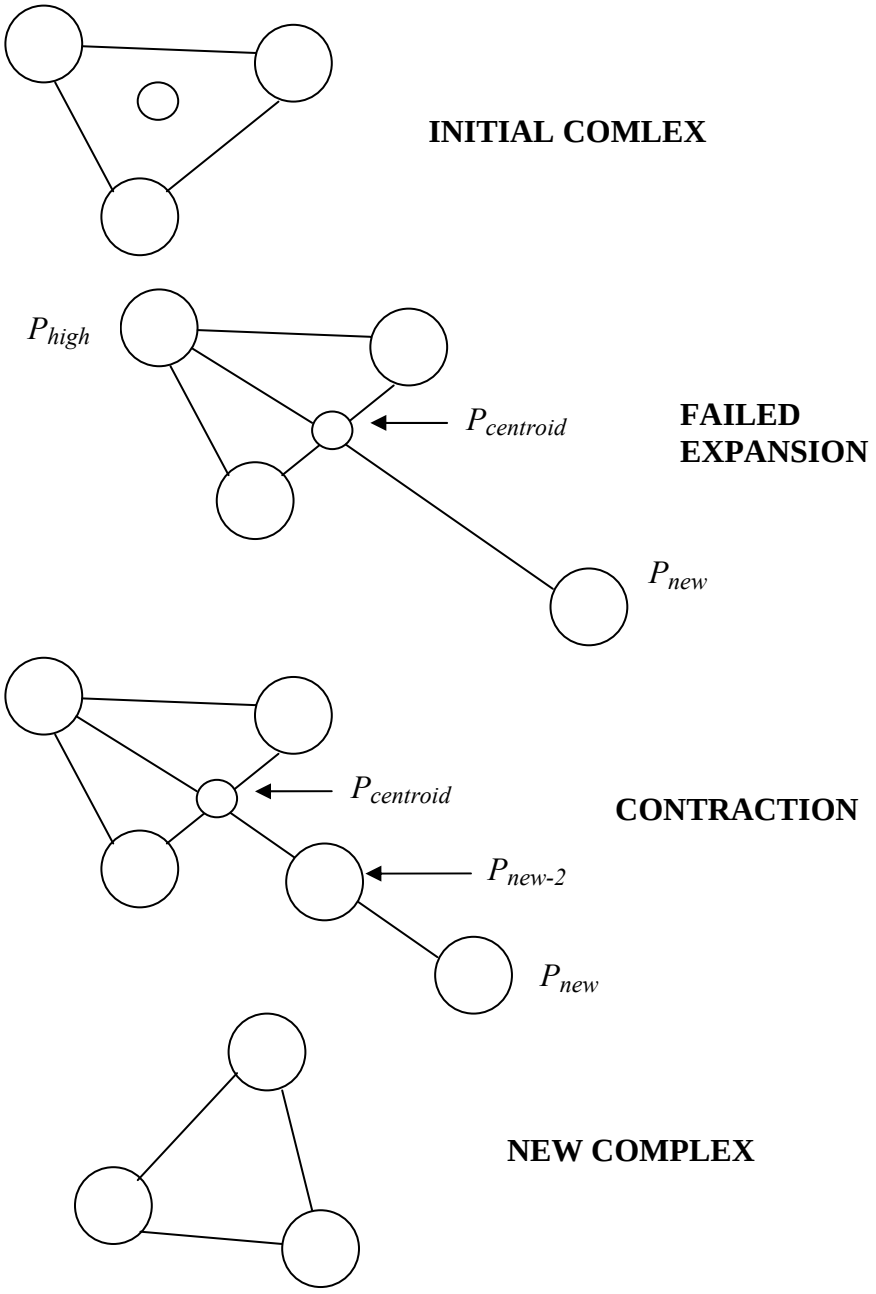


Figure 2-7. Complex Contraction in the Box Complex Method

2.3.2.3.2 Shuffled Box Complex Method

The original Box Complex method of optimization is modified by incorporating the concept of multiple complex evolution and complex shuffling. In the Shuffled Box Complex method, instead of generating one complex of solution points, multiple complexes are generated that move in the direction of function minimization simultaneously via different search directions. After a specified number of generations (iterations), the points constituting the multiple complexes are shuffled randomly and reassigned to the complexes. The new complexes then continue to move towards the constraint boundary in the direction of function minimization. Such a shuffling process will ensure that information contained in the sample is efficiently and thoroughly exploited. It will make the search process more robust and diverse by mixing information between complexes. Shuffling will also enhance survivability by a sharing of the information between different solution sets. This process of shuffling can be considered evolutionary in the sense that communities are made to mix during the search process causing a sharing of information similar to the genetic operations of crossover and mutation in the case of evolutionary optimization methods such as a genetic algorithm. The shuffling continues until a specified convergence criterion is met or the specified number of generations is over. The concept of evolving multiple complexes and complex shuffling was first developed by Duan et al. (1993) in their Shuffled Complex Evolution (SCE) approach for global minimization. The difference between SCE approach and the proposed Shuffled Box Complex method lies in the specific application. The SCE approach was applied to an unconstrained optimization problem and a technique known as the competitive Complex evolution (CCE) was used to evolve each individual complex in the search space. In contrast, the Shuffled Box Complex method has been developed for constrained optimization problems in which the individual complexes are evolved using the original Box Complex method of optimization with the provision for handling inequality constraints through complex contraction.

2.3.2.4 Evolutionary Methods

Evolutionary computation is the study of computational systems which use ideas and get inspiration from natural selection and adaptation. The primary aim of evolutionary computation is to study and develop robust and efficient computational systems for solving complex real world problems. Sarker et al. (2002) reports that evolutionary optimization is the most active and productive area of evolutionary computation as measured by the number of successful applications and resulting publications in this area. All evolutionary or heuristic search methods are characterized by a population of solutions that evolve to better solutions through a process or mechanism that is analogous to the process of natural selection (Goldberg, 1989). There is no formal mathematical proof for evolutionary methods but they have been proven to be superior to traditional optimization methods, particularly in case of nonlinear, non-convex, multi-modal problems (Muleta, 2003).

Evolutionary computation consists of four major branches namely 1) evolutionary programming, 2) evolution strategies, 3) genetic algorithms, and 4) genetic programming. Of these four, the first three types of algorithms have been collectively grouped under evolutionary algorithms (EAs) by more and more researchers (Sarker et al. 2002). All these three types of evolutionary algorithms namely evolution strategies, evolutionary programming, and genetic algorithms use similar computational framework. This is shown in Figure 2-8.

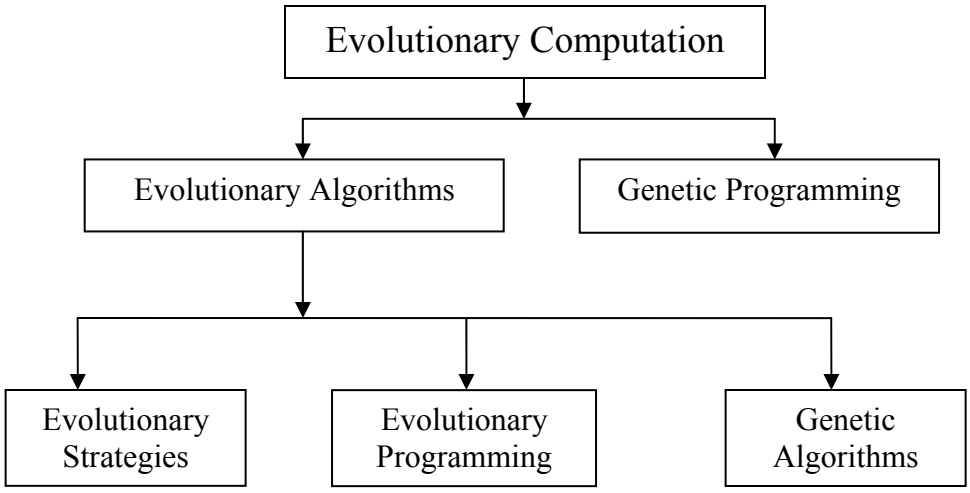


Figure 2-8. An Overview of Evolutionary Computation Methods

Evolutionary strategies were first proposed by Rechenberg and Schwefel in 1965 as a numerical optimization method and did not include the concept of a "population". The "population" concept was introduced into evolution strategies later (Schwefel, 1981; Schwefel, 1995; Sarker et al. 2002).

Evolutionary programming was first proposed by Fogel (1962) as a way to achieve artificial intelligence and since then several examples of evolving finite state machines were demonstrated (Fogel et al. 1966). Since the late 1980's, it has been used to solve various combinatorial and numerical optimization problems (Sarker et al. 2002).

Genetic algorithms (GAs) were first introduced by Holland (1975) and his students (DeJong, 1975). Genetic algorithms are mostly used as global optimization methods for combinatorial or numerical problems. GAs are probably the most well-known branch of evolutionary computation (Sarker et al. 2002).

Genetic programming (GP) is a branch of genetic algorithms (Koza, 1992). It should be noted that GA is not a model-building tool and has been used traditionally for finding optimal values of parameters or decision variables of existing models. Thus while GA

use a string of numbers to represent the solution, GP has the capability to create computer programs or models that can turn inputs to outputs from specified building blocks such as mathematical operations and variables. The output from a GP is an empirical model used for approximation whereas the output from a GA is the optimal values of the parameters or decision variables of a known empirical model (Alvarez et al, 2000).

2.3.2.4.1 Framework of Evolutionary Algorithms (EAs)

All evolutionary algorithms have two prominent features that separates them from other search methods and these include 1) they are population based, and 2) there is communication and exchange of information between individuals in a population. This types of communication and information exchange is a result of selection and/or recombination in evolutionary algorithms. A general framework of evolutionary algorithms is given in Figure 2-10. Note that the search operators for instance in the case of genetic algorithms will be the genetic operators such as generation, crossover, and mutation. These operators are used to produce off-springs (new individuals or solution vectors) from parents (existing individuals).

The framework given in Figure 2-9 is a general framework for all evolutionary algorithms. Different algorithms vary from one another in the different representation of individuals and different methods of implementing fitness evaluation, selection, and search operators (Sarker et al. 2002). The next subsection will give an overview of genetic algorithms for use as a global optimization technique in this research.

1. Set $i = 0$;
2. Generate the initial **population** P(i) at random;
3. REPEAT
    a. Evaluate the **fitness** of each individual in P(i);
    b. **Select** parents from P(i) based on their fitness;
    c. Apply **search operators** to the parents and produce generation P(i +1);
4. UNTIL the population converges or the maximum time is reached

Figure 2-9. General Framework of Evolutionary Algorithms (Sarker et al. 2002)

Of the three EAs described above (Figure 2-8), this research will investigate the utility of genetic algorithms (GAs) as an optimization method for application to the watershed management problem. GAs are described in detail in the following section.

2.3.2.4.2 Genetic Algorithms (GAs)

GAs are a subset of EAs that mimic biological principles (Darwin's theory of evolution) to optimize highly complex functions. The method was developed by John Holland (1975) in the 1960s and 1970s but was popularized by one of his students, David Goldberg, who applied it to solve a difficult problem in engineering involving the control of gas pipeline transmission for his PhD dissertation (Haupt and Haupt, 1998). A genetic algorithm (GA) is a stochastic numerical search procedure inspired by biological evolution and natural selection. GA is used in cross breeding trial solutions and allowing the fittest solutions to survive and propagate to successive generations. GA deals with a population of individual solutions which undergo constant changes by means of genetic operations of *reproduction*, *crossover*, and *mutation* (Goldberg, 1989). GA can be viewed as a search procedure where the search process is controlled by the fitness of the solution vector (Burn and Yulianti, 2001). A solution in GA is represented as a string of

decision variables (also referred to as chromosome) that evolves through generations to further improve its fitness. A simple GA consists of the following steps (Burn and Yulianti, 2001) as shown in Figures 2-10 and 2-11:

```
{
        Initialize population;
        Evaluate population;
        While TerminationCriteriaNotSatisfied
        {
                Select parents for reproduction;
                Perform crossover and mutation;
                Evaluate population;
        }
}
```

Figure 2-10. A simple Genetic Algorithm

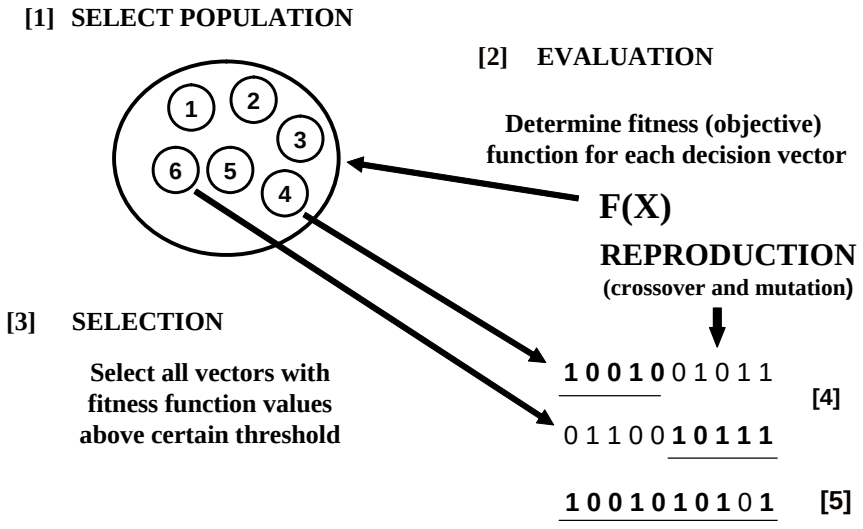


Figure 2-11. Steps in a simple Genetic Algorithm

1. Select an initial population of solution vectors or strings.

   Each of these vectors (also called *chromosomes*) is defined by a sequence of decision variables, known as *genes* in GA terminology. These can be represented as a string of binary or real numbers or integers. In case of binary representation of genes, the length of each chromosome is defined by the user (Muleta, 2003).

2. Evaluate the fitness of each string.

   For each of the solution chromosomes chosen during the random search, a measure of fitness (which corresponds to an objective function value) is evaluated. All solution chromosomes in the initial population are referred to as species of the first generation. Their chance of survival depends on the values of their fitness (Muleta, 2003).

3. Select strings from the current population to mate.

   The chromosomes of the first generation are then ranked in an ascending order (for minimization problems) to determine the ones that will get the chance to mate and produce off-springs. The ones with higher fitness values (low objective function value) will have the greater chance to survive to the next generation (Muleta, 2003). This process of choosing mates is called *selection*.

4. Perform crossover for the selected strings.

   Once the chromosomes for mating (parents) are selected, there is exchange of information between the genes of the selected parents that gives rise to off-springs. The mechanism of creating new individuals by assigning them genes of the parents is called *crossover*. In this manner, new individuals will replace the ones that had the worst fitness values in the previous generation. There are many ways in which crossover can be performed and using different methods generates new types of GAs (Muleta, 2003).

5. Perform mutation for the selected string elements.

   To bring diversity in the new individuals created after crossover operation and to make sure that the search is not confined to the genes brought by the initial population selected randomly, the operation of *mutation* is performed. In mutation, a certain percentage of chromosomes (often 3 to 10 percent) are selected and their genes are altered at a randomly selected location. This will change the genes of the selected chromosomes and prevents the GA from being trapped in local minima.

6. Repeat steps 2-5 for the required number of generations.

   The process of evaluating fitness, selection, crossover, and mutation is carried over and over in a cyclic manner until the GA converges to an optimal solution that meets user's criteria or the number of specified generations is over. Also, if the solution vectors are not getting any better in successive generations, the GA search process can be terminated.

There are many advantages of using GAs over traditional optimization methods and some of these are summarized as follows:

- They do not require derivative information,
- They can deal with a large number of parameters,
- Their concept is easy to understand.
- They support multi-objective optimization,
- They are good for noisy environments,
- They are well suited for parallel computers,
- They provide a population of solutions and not just one solution,
- They are capable of searching simultaneously from a population of solutions,
- They are known to be successful in optimizing complex, non-linear, and noisy functions for which other traditional methods fail.

The most important advantage of GAs as stated by Muleta (2003) is their ability to work for functions that are not easy to describe mathematically such as the hydrologic and water quality processes occurring in a watershed. It is very difficult to obtain a well-behaved mathematical relationship between the inputs and outputs involved in such processes and GAs are very well suited for such complex and non-linear problems. GAs has been successfully applied to a variety of problems in water resources engineering and management as presented in Muleta (2003). Consequently, there are numerous publications on the use of GAs as global optimization tools by researchers covering a broad spectrum of water resources engineering and management areas. It is therefore not feasible to list a reference to all of these publication but a some of these include Hilton

and Culver (2000), Nishikava (1998), Ritzel et al. (1994), Reis et al. (1997), Wang (1991), McKinney and Lin (1994), Esat and Hall (1994), Oliveira and Loucks (1997), Wardlaw and Sharif (1999), Savic and Walter, (1997), Hellman and Nicklow, (2000), Reddy and Ormsbee (2002).

It should be noted however that GAs are not the answer to every optimization problem and they too like other traditional optimization problems have certain limitations. Effort should be made to understand such limitations and keeping them in view one should make a decision on when and how GAs can be used for a particular application. For instance, for well behaved response functions, other traditional methods are known to be more efficient and they can outperform GAs in finding the optimal solutions (Haupt and Haupt, 1998). It should also be noted that GAs are technically only applicable to unconstrained problems. Another shortcoming of the method is its significant computational expense, particularly in cases where the complex objective function evaluation may require significant time. Finally, it should be realized that GA are a heuristic optimization technique and does not guarantee a globally optimal solution (Muleta, 2003). But as pointed out by Nicklow (2000), the fact that the majority of literature on GAs demonstrates its ability to obtain global or near global optimal solution continue to make it a favorable choice for researchers. The benefits of using the GA technology should meet the key requirements of the application in hand for GAs to be effective optimization tools.

2.3.2.4.3 Genetic Algorithms for Constrained Optimization

As indicated above, GAs are directly applicable only to unconstrained optimization problems. In the application of GAs to constrained nonlinear optimization problems, a particular solution vector (*chromosome*) can violate certain constraints of the problem formulation and can thus result in infeasible solution sets. In the recent years, different methods have been proposed for handling constraints by GAs. These can be grouped into the following categories (Yeniay, 2005):

1. methods based on preserving feasibility of solutions,
2. methods based on penalty functions,
3. methods based on a search for feasible solutions, and
4. hybrid methods (Michalewicz and Schoenauer, 1996).

Of these four methods, penalty function methods are the most popular methods used for constrained optimization problems using a GA. These methods transform a constrained problem into an unconstrained problem by imposing a penalty on the infeasible solution. This is done by adding to the objective function value a positive value (penalty) which reduces the fitness value of such infeasible solutions (Yeniay, 2005). This decreases the chances of the solution to have a significant impact on the offspring solutions as they evolve in future generations. Both static and dynamic penalties can be applied when using GAs for constrained optimization (Sarker et al. 2002). Comparative studies about penalty function methods in GA can be found in Kuri-Morales and Gutierrez-Garcia (2001), Miettinen et al (2003), and Yeniay (2005). The use of penalty functions in using GAs for constrained optimization can be considered as a drawback as they can require extensive fine tuning and parameter estimation. This disadvantage of GAs was one of the motivator for developing the Shuffled Box Complex method for the constrained optimization problem in this research which does not require penalty functions.

CHAPTER 3
MATHEMATICAL MODELS FOR WATERSHED MANAGEMENT

3.1 Introduction

In this chapter, an overview of the types of mathematical models and the methods of analysis used in mathematical models is presented. This will lead to some applications of mathematical models used for watershed management. In particular, this chapter will provide a brief discussion on the two commonly used approaches (types) of mathematical models (also referred to as simulation models) namely, 1) deductive or mechanistic models and 2) inductive or empirical models. This will be followed by a discussion on the analysis methods used in the development of these two types of modeling approaches. In the context of watershed simulation models, both deductive and inductive watershed models will be discussed. An overview of some of the available deductive watershed models available to the public is given in the context of deductive watershed models for hydraulic, hydrologic, and water quality modeling.

This research will evaluate the development of effective watershed response models for processes occurring in an urban watershed that can be used in an optimal management framework for linkage with efficient optimization algorithms. The concepts and methods discussed in this chapter are therefore important and will provide a good platform for understanding the work described in the future chapters.

3.2 Mathematical Modeling

Mathematical modeling is the process of creating a mathematical representation of some phenomenon in order to gain a better understanding of that phenomenon. It is the use of mathematics to describe real world phenomena, test ideas, and make predictions about a real world process being modeled. It can thus be seen as a process that attempts to match observation with symbolic statement. "Generally the success of a model depends on how

easily it can be used and how accurate are its predictions." (Edwards and Hamson, 1990, p.3).

The analysis, design, or management of any real world process is facilitated through the use of systems approach. In systems analysis (approach) a physical or engineered system is represented in a simplified form through the construction and use of a mathematical model (Figure 3-1). Such models represent a systematic organization of a system's knowledge developed for some kind of planning, engineering, or scientific purpose. From a watershed management perspective, the most important subsystem is the watershed system. Scientists and engineers develop and use descriptive models for the purpose of describing such a physical system or sub-system and for the purpose of predicting the behavior of such a system in response to a given stimulus or loading.

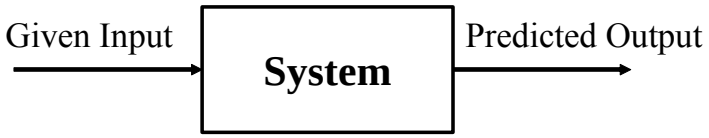


Figure 3-1. Systems Approach

A mathematical model can be used to represent a wide range of systems (Sinha, 1991; and Mays, 1997) such as:

- Static and dynamic systems
- Linear and nonlinear systems
- Time-varying and time-invariant systems
- Deterministic and stochastic systems
- Continuous-time and discrete-time systems
- Lumped-parameter and distributed-parameter systems

Depending on the type of system being modeled, the resulting mathematical model may be classified accordingly. Most real world systems are dynamic, nonlinear, time-varying,

and stochastic, and often require the development of complex models to fully and accurately represent them.

It is worth mentioning here that computer models do not solve problems but only provide guidance to the user who then utilizes the information in the most beneficial way. Mathematical modeling plays a very useful role in the design, analysis, and management of a system through (Lund and Palmer, 1998):

- Furthering understanding of the problem.
- Defining solution objectives.
- Developing promising alternatives.
- Evaluating alternatives.
- Providing confidence in solutions.
- Providing a forum for negotiations in the final decision making.

The purpose of most models is to reproduce consistently the observable phenomena that are of significance for a particular problem. For example, the purpose of a dissolved oxygen water quality model is to reproduce in time and space the dissolved oxygen patterns observed at a particular site taking into account the effects of flows and pollution loads, etc. Models can be used to assist in real-time decision-making or evaluate a physical or biological system under past, present, and future conditions (BDMF, 2000). For water-related areas, mathematical modeling can be applied to the following (BDMF, 1997):

- Fisheries, aquatic biology, and habitat health
- Groundwater
- Hydrodynamics
- Hydrology, hydraulics, and irrigation
- System operations and real-time management
- Water quality and Watershed Management
- Water resources planning

3.3 Types of Mathematical Models

Mathematical models represent existing or hypothesized knowledge of how a system works and may be classified on the basis of the origins of such knowledge. Two different strategies are typically employed in building a mathematical model. These include either a deductive or mechanistic approach or an inductive or empirical approach. Deductive models are based on the basic fundamentals of physics and chemistry governing a process or system, while inductive models are data driven models that are based more directly on field or laboratory observations. The question of "which type of model to use?" has been asked ever since modeling of systems has been in place. Numerous models have been developed in the quest to find the best approach or strategy to model different systems or processes. It can be safely said that no one model can fully explain the complexity of the real world and that is the reason why modelers continue to develop models of varying complexity, generality, and validity. Thus Beck (1985) has stated that "Different types of models are appropriate for solving different kinds of problems; there is no universal model for solving all manner of problems; comprehensiveness and complexity in a simulation are no longer equated with accuracy; and there is a healthy mood of critical questioning of the validity and credibility of water quality models". Both empirical and mechanistic models have found various and successful implementations and developments in different scientific areas. When comparing the potential of the empirical and mechanistic approaches, it is recommended to select models on both extremes of the empirical/mechanistic scale, (i.e., empirical models with as little mechanistic assumptions as possible and mechanistic models with as few empirical features as possible) (Nestorov et al. 1999).

Different analysis methods are used to construct deductive and inductive models. For deductive models these methods may consist of different numerical schemes (e.g. finite difference or finite element methods) to solve the underlying governing mathematical equations representing the process or system being modeled. Conversely, inductive models are constructed using methods that relate a given set of independent variables to a given set of dependent variables (e.g. regression).

3.4 Deductive Mathematical Models

Most traditional mathematical models used in planning and/or design are deductive or mechanistic models. These are also referred to as physically or process based models. Such models rely on the fundamental laws of physics and chemistry that govern a particular process or system under study. Some examples of deductive modeling approach are given as follows (BDMF, 2000):

- Use of conservation of mass to derive models of the operation of river-reservoir systems;
- Use of conservation of mass, momentum, and energy with channel geometries and bed elevations for hydraulic routing;
- Use of principles of advection and dispersion for contaminant transport modeling;

Mechanistic or deductive models commonly consist of a set of fundamental governing equations representing conservation of mass, energy, and momentum, reaction kinetics of various pollutants, etc. In most cases, these equations are either partial differential equations or ordinary differential equations. Except for a few particular cases, remote from the real world, a general analytical solution of the complex set of differential equations cannot be found (Ciriani et. al., 1977). These governing equations have initial or boundary conditions, and can be solved by several numerical schemes.

Deductive models can be applied in different ways depending on the manner in which the input and output of the model is used. These include 1) deterministic, 2) parametric, and 3) stochastic. In deterministic models, all model parameters are assumed to have discrete values that are used in the governing equations of the process being modeled to obtain model outputs. In parametric models, model parameters are obtained by calibration using observed model inputs and outputs. In stochastic models, probability distributions of model parameters are obtained for use in the model to obtain a probability distribution of the model output.

3.4.1 Analysis Methods for Deductive Models

Once the mathematical form of a deductive model (set of differential equations) has been specified, the numerical method to solve the model equations must be found. Often, particularly for complex models, the solution method for the model equations will require testing to ensure that the numerical solutions are correct for the intended types of problems and modeling objectives. Concerns about accuracy and stability of a particular numerical scheme can be addressed by comparing the numerical solutions with (1) analytical solutions available for special cases or (2) solutions from trusted numerical solution methods (BDMF, 2000).

The key to various numerical methods is to convert the partial or ordinary differential equations that govern a physical phenomenon into a system of algebraic equations. Different techniques are available for this type of conversion. There are five commonly used, closely related, numerical methods for solving differential equations namely 1) finite difference methods, 2) finite element methods, 3) collocation methods, 4) method of characteristics, and 5) boundary element methods (Pinder, 1983). In applications of water resources systems modeling, the finite difference and finite element methods are more popular than any of the other methods (Tufail, 1995). A brief description of these two methods is given as follows.

3.4.1.1 Finite Difference Method (FDM)

The finite difference has been a very familiar and popular approach for modeling of physical processes in engineering. The method consists of replacing directly the governing partial derivatives by quotients of finite differences. This results in a system of algebraic equations that are solved, after imposing the boundary conditions, for the unknowns at discrete mesh points of the region being analyzed. Most common finite difference representations of derivatives are based on Taylor's series expansion (Anderson, 1995). There are several practical reasons for the popularity of this method as summarized below (Pinder, 1983):

- Finite difference methods are simple and conceptually straightforward.
- The fundamental concepts are readily understood and do not require advance training in applied mathematics.
- The form and algebraic simplicity of the equations arising from difference approximations have led to the development of several efficient algorithms for their solution.

Finite difference methods can fall into one of the two approaches namely explicit or implicit as discussed below.

3.4.1.1.1 Explicit Finite Difference Methods

In an explicit approach of finite difference method, each difference equation (representing a governing differential equation) contains only one unknown and can therefore can solved in a straight forward manner explicitly for the unknown(s). This is the simplest of the approaches of solving difference equations. A disadvantage of the explicit methods is that they are not unconditionally stable, meaning that for a given spatial grid length Δx, the corresponding temporal interval Δt must be less than some limit imposed by the stability constraints. This may in some cases lead to a very small Δt thus leading to longer run times in the computation of the solution over a given simulation time.

3.4.1.1.2 Implicit Finite Difference Methods

In an implicit approach of finite difference method, there are more than one unknown in the resulting difference equations and these must be obtained by means of simultaneous solution of the difference equations applied at all points of the grid representing the discretization. In terms of stability, implicit methods are unconditionally stable and thus they allow for using larger computational time steps (Δt). However, the use of larger Δt can lead to larger truncation errors in the solution. Due to the simultaneous solution of a large system of equations, the implicit approach is more complex in terms of

computations and is relatively more difficult to program than the explicit approach (Anderson, 1995).

3.4.1.2 Finite Element Method (FEM)

The finite element is an approximation procedure for solving partial differential equations of boundary and/or initial value type in engineering and mathematical physics. This is a very powerful, modern computational tool for solving engineering problems, and has gained wide acceptance in the area of computational fluid mechanics (Stasa, 1985). The procedure employs subdivision of the solution domain into many smaller regions of convenient shapes, such as triangles and quadrangles, and uses approximation theory to quantize behavior on each finite element. The approximation functions are derived using the basic idea that any continuous function can be represented by a linear combination of algebraic polynomials. Thus, over each finite element, the physical process is approximated by functions of desired type (polynomials or otherwise), and algebraic equations relating physical quantities (unknowns of the governing differential equations) at selected points (nodes) of the element are developed (Reddy, 1993). These element equations are collected together to form a global system of algebraic equations including a proper accounting of the boundary conditions. Finally, the nodal values of the dependent variables (unknowns) are determined from the solution of this global matrix equation system (Baker, 1983).

The most distinctive feature of the FEM that separates it from other numerical schemes is the division of a given domain into much simpler sub-domains, called *finite elements.* Any geometric shape that allows computation of the solution or its approximation at selected points (referred to as nodes) of the sub-domain, qualifies as a finite element. The use of interpolation functions to define the unknown variables throughout the problem domain is an important concept that distinguishes the FEM from the more popular FDM. In the FDM, the unknowns are defined only at the nodal points, whereas in the FEM, the unknown variables are defined throughout the problem domain in a piecewise fashion over the individual elements. This characteristic of the FEM permits

the application of variational or weighted residual principles. One of the main advantages of the FEM over other numerical methods, including the FDM, is the fact that FEM can handle irregular geometries routinely. However, for one-dimensional problems this is not a significant factor. Another significant advantage of the FEM is the easy handling of the variable spacing of the nodes. Also, the FEM has the capability with which non-homogeneous and anisotropic materials can be easily handled, a feature not available easily with the FDM. Lastly, the implementation of higher-order elements in the FEM makes it more preferable than the FDM (Stasa, 1985). This can allow modeling of critical regions of the domain more precisely, thus improving the accuracy of the approximate solution. Some disadvantages associated with the FEM include the necessary use of digital computers and expensive software. In the end, the choice of a particular method (FEM, FDM, or others) used in a particular application depends on the complexity of the problem, and the user's familiarity with the different methods that can be used (Tufail, 1995).

3.4.2 Deductive Watershed Models

Deductive watershed simulation model provide tools for simulating the movement of precipitation and pollutants from the ground surface through pipe and channel networks, storage treatment units, and finally to receiving waters. Both single-event and continuous simulation may be performed on catchments having storm sewers and natural drainage, for prediction of flows, stages and pollutant concentrations. EPA and state agencies have emphasized watershed-based assessment and integrated analysis of point and non-point sources of pollution (EPA, 1997). As a result, models are being increasingly used to evaluate a wider range of pollutant transport and receiving water impacts issues.

Deductive watershed models play an important role in linking sources of pollutants to receiving water bodies as source loads. Deductive watershed models are driven by precipitation, land use, impervious areas, slope, soil types, and drainage area. A deductive watershed model for a watershed can simulate both water quantity and water quality processes such as interception soil moisture, surface runoff, interflow, base flow,

snow pack depth and water content, snowmelt, evapotranspiration, ground-water recharge, dissolved oxygen, biochemical oxygen demand (BOD), temperature, pesticides, conservatives, pathogens, sediment detachment and transport, ammonia, nitrite-nitrate, organic nitrogen, orthophosphate, and organic phosphorus. Any period from a few minutes to hundreds of years may be simulated in such models. Such models are used to assess the effects of land-use change on different processes, stream flow routing, reservoir operations, point and non-point source treatment alternatives, flow diversions, etc.

Different types of deductive models of varying complexity can be developed for a watershed. For a given watershed of sufficient complexity, a general mathematical model can be represented as given in Figure 3-2.

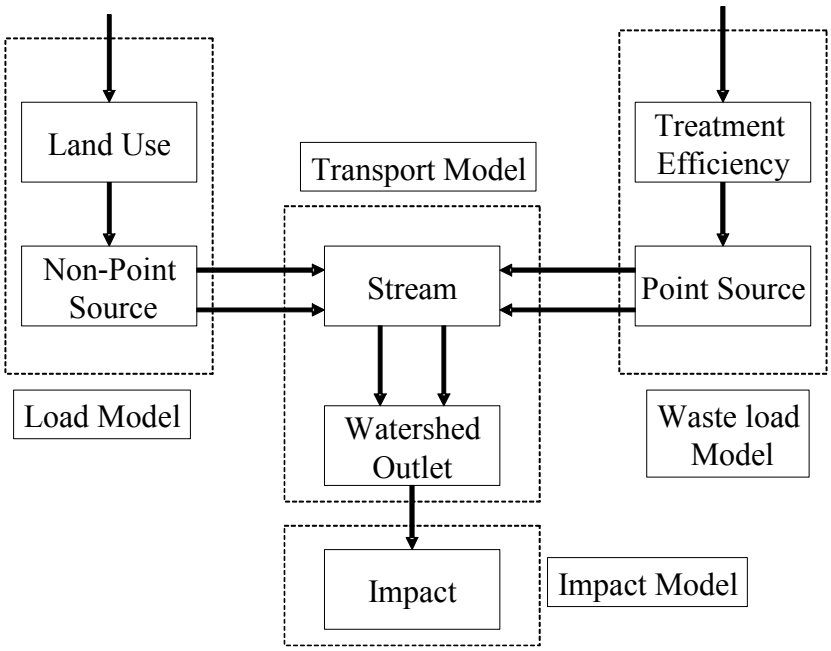


Figure 3-2. Deductive watershed model

The following three broad categories of models are typically developed for a watershed management system:

1. Watershed response models,
2. Transport models, and
3. Receiving water models.

In general, a comprehensive watershed model such as shown in Figure 3-2 can be used to simulate water quality contributions from both point and non-point sources of pollution and evaluate their impacts on the receiving waters. From a practical perspective, the transport model as shown in Figure 3-2 will usually be combined with either the watershed response model or the receiving water model. Thus we can categorize watershed simulation models (and thus water quality models) into two main and commonly used categories given as follows (USEPA, 1997):

- Watershed loading models that simulates the generation and movement of pollutants from the source to a discharge point in the receiving waters, and
- Receiving water models that simulate the movement and transformation of pollutants through water bodies such as lakes, streams, rivers, and estuaries.

These models are used for different purposes allowing scientists and engineers to determine the assimilative capabilities of the water body, determine level of best management practices, etc. Figures 3-3 and 3-4 give an overview of these two types of models supported by EPA for use in watershed assessment and water quality modeling and these range in complexity and applicability (EPA, 1997). Three different types of loading models are given in Figure 3-3. These include 1) simple models, 2) mid-range models, and 3) detailed models. Simple models are derived from empirical relationships between physical characteristics of the watershed and pollution export. They can often be applied using a spreadsheet program or hand-held calculator. The mid-range models are used to evaluate pollution sources and impacts over broad geographical scales. These types of models are a compromise between simple and detailed models. The detailed models best represent the watershed processes affecting pollution generation. These types of models are used to identify causes of problems rather than simply describing the overall conditions (EPA, 1997).

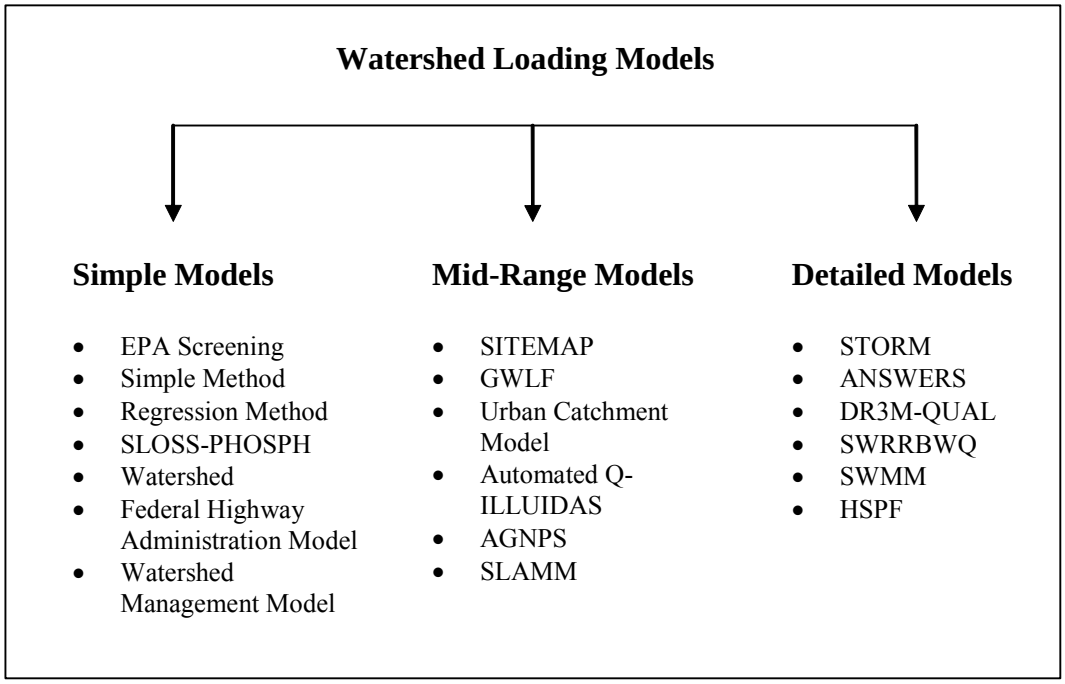


Figure 3-3. Overview of Watershed Loading Models (USEPA, 1997)

The receiving water models are classified as either hydraulic models or water quality models as given in Figure 3-4. Under these two classes, four different types of receiving water models are given in Figure 3-4. These include 1) hydrodynamic models, 2) dynamic water quality models, 3) steady state water quality models, and 4) mixing zone water quality models. Hydrodynamic models simulate the "dynamic" or time-varying features of water transport and are used to represent water movement in rivers, lakes, streams, reservoirs, estuaries, near-coastal waters, and wetland systems (EPA, 1997). Dynamic water quality models are used to simulate time-varying features of the fate and transport of water quality constituents. Steady-state models do not have the capability to simulate the time-varying features of the fate and transport of water and pollutants, and use constant values of input variables to predict constant values of target variables. Lastly, mixing zone models are often referred to as "near field" models and are mostly used to assess limited areas of contaminant mixing in the vicinity of a wastewater discharge. These models can be used in the development of discharge permits as well as TMDLs (EPA, 1997).

Interested readers are encouraged to refer to USEPA (1997) in which the detailed characteristics of each of these models is presented. While some deductive models can be commercially purchased, others are public domain software developed mainly by governmental agencies for public use. Additional information on the use and application of the above mentioned models can be found on the EPA web site (http://www.epa.gov/athens/wwqtsc/index.html) dedicated to providing technical support on watershed and water quality modeling (EPA, 2005).

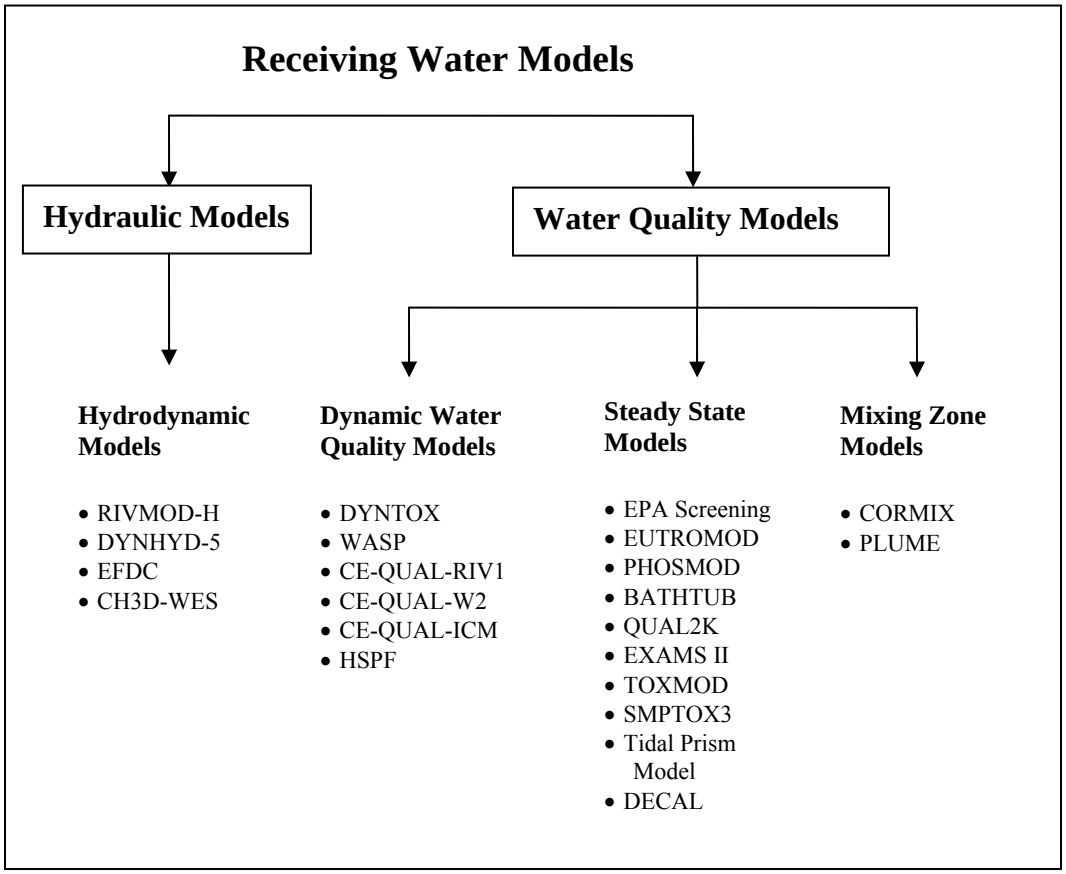


Figure 3-4. Overview of Receiving Water Models (USEPA, 1997)

3.5 Inductive Mathematical Models

An inductive or empirical model is based on data and is often used to predict, not explain, a system. An empirical model consists of a function that captures the trend of the data.

The equations and calibrations of inductive models rely (more directly) on field or laboratory data, or empirical observations. It is important to understand the use of an inductive model for a particular application. It has been found that an inductive model may be a very good "predicting tool" but may not provide a good cause and effect relationship between all input and output variables of the model. This is due to the fact that inductive models are essentially data fitting models and it is sometimes difficult to capture the cause-and-effect dynamics of the process or processes being modeled. Regardless, inductive or data-driven models are becoming more and more popular due to their ease of use and simplicity as substitutes for more process-based models in a number of applications. For instance, inductive models may be preferred where 1) computational expense is a critical issue, 2) the process-based deductive model is over parameterized and cannot be adequately calibrated, and 3) budgetary constraints do not allow for a complex deductive model. Inductive models may also be more favorable in the real time control of highly dynamic systems when quick and effective management decisions are needed to facilitate reliable and safe operation of the systems. For instance, in the real time control of combined sewer systems, such models can serve as an effective management tool for managers to make quick operational decisions during storm events. The use of deductive models in such scenarios may be restricted by their inability to yield rapid response to dynamically changing conditions.

Examples of inductive models range from simple linear regression models to more complex nonlinear models based on artificial neural networks (ANNs). Both linear and non-linear inductive models can be used to fit a mathematical model to a given data set in order to represent a process. By definition, regression based models are restricted in the sense that specific form of the function being sought has to be specified such as n-order polynomial, an exponential function, etc. In cases where the dominant functional relationships of the data sets cannot be precisely pre-determined, other methods must be investigated (Tufail and Ormsbee, 2006).

3.5.1 Analysis Methods for Inductive Models

Analysis methods for inductive models refer to the particular technique or method used in the development of such models. Examples of inductive models range from simple linear regression models to more complex nonlinear models based on artificial neural networks (ANNs). More recently, inductive models derived using evolutionary and biological principles are becoming increasingly popular. Genetic algorithms (GAs) and artificial neural networks (ANNs) are two such evolutionary methods that have found numerous applications in the development and application of inductive models to real world engineering processes. GAs represents a class of probabilistic search procedures that use computational methods based on natural evolutionary processes (Goldberg, 1989). ANN-based models represent a digital model of the functional processes of the human brain (Zurada, 1992). ANNs can also be thought to be evolutionary in way that the training weights in the network evolve or are optimized to improve system performance. Each of these models has been found to be particularly powerful in those applications when a large number of solutions need to be evaluated over a shorter period of time. Regression techniques are the simplest form of inductive models being used in scientific research and will not be discussed in any detail here. A detailed description of the increasingly popular evolutionary techniques used for building effective nonlinear inductive models for a response function is given in the sections to follow. These include ANNs, a GA-based technique called genetic programming (GP), and genetic functions (GFs).

3.5.1.1 Artificial Neural Networks (ANNs)

3.5.1.1.1 Introduction

Recent advances in computational sciences have seen ANNs receiving a great deal of attention as a powerful tool of computation and knowledge representation. This excitement is partially due to the ability of ANNs to imitate the brain's ability to make decisions and draw conclusions. Essentially, ANN is a mathematical model constructed so as to approximate the basis functions associated with a biological neuron. In other words, it is a digital model of the human brain, and it imitates the way a human brain works. It consists of a highly interconnected network of several simple processing units

called neurodes or neurons. ANNs work by creating connections between processing elements (the computer equivalent of neurons) and consist of an input layer of elements or neurons, a hidden layer or layers of neurons, and an output layer of neurons (Figure 3-5). The organization and weights of these connecting elements determine the output.

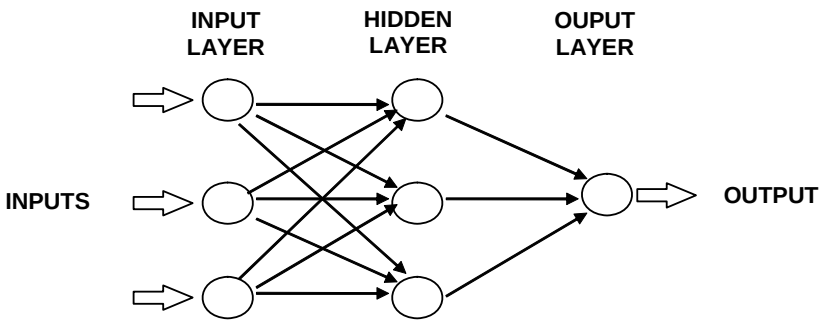


Figure 3-5. Architecture of a simple ANN

Each connection from one neuron (say A) to another neuron (say B) possesses a numeric weight representing the strength of connection between the two neurons. A high positive strength means that when A is active B should also be active. A near zero strength means that "A" being active will have little effect on "B". Other valuable characteristics of an ANN include 1) their ability to produce correct or nearly correct responses when presented with partially incorrect, incomplete, or noisy information in the form of input data, 2) their ability to generalize rules from the patterns presented on which they are trained, and apply these rules to new set of input data (Jain, 1994), and 3) their ability to extract the relationship between model inputs and outputs without knowing the underlying physics of the process being modeled (Muleta, 2003).

3.5.1.1.2 History of ANNs

Jain (1994) and Muleta (2003) have described the history of ANNs in their work which can be summarized as follows:

- The origin of ANNs dates back a century ago when William James published a book, Principles of Psychology (James, 1890) in which some of the principles of correlational learning and associated memory were stated. He proposed the basic notion of a neuron's ability to be a function of the sum of its inputs, with the past correlation history contributing to the strengths of interconnections.
- In 1943, McCulloch and Pitts (1943) published a ground breaking paper in which they derived theorems related to models of neuronal systems by emulating the human brain's information processing system.
- Rosenblatt (1958) presented a paper in which the neural network structure of a perceptron was defined. This led to the first perceptron model for implementation on an IBM computer in a study conducted at the Cornell Aeronautical Laboratory (Eberhart and Dobbins, 1990). This also led to the development of supervised and unsupervised learning algorithms as seen in ANNs in the form of back propagation and Kohonen networks (Jain, 1994).
- The popularity of ANNs as powerful and effective computation tools were realized after the efforts of Hopfield (1982) and Rumelhart et al. (1986). The latter provided an excellent description of the basic anatomy of ANNs leading to the basic architecture and learning algorithm known as the back propagation method.
- Since the work of Hopfield (1982) and Rumelhart et al. (1986), there have been numerous applications of ANNs in various fields of science and engineering such as physics, biomedical engineering, robotics, image processing, sound recognition, finance, and many others (Muleta, 2003).

3.5.1.1.3 Structure of a Back Propagation ANN

Back propagation ANNs are the most commonly used networks by engineers and scientists (Jain, 1994). This can be attributed to its simple structure and its method of supervised learning that can be controlled externally depending upon the specific application. ANN-based inductive models developed in this research use back

propagation neural networks and therefore only these type of neural network models are discussed in detail here..

Back propagation ANNs derive their name from the method in which they learn (i.e. the errors are propagated back from the output neurons) (Rumelhart, 1986). Figure 3-6 shows the structure of a simple 3-layer back propagation ANN model with an input layer (four neurons or inputs), a hidden layer (four neurons), and an output layer (two neuron or outputs). The number of neurons in each of these layers can vary based on the specific application. Also, the number of hidden layers varies based on the complexity of the model. The number of hidden layers and the number of neurons in each hidden layer are often varied to train ANN models in order to achieve optimal training. The neurons in an input layer receive input (also called activation) from an external source and then send output to a hidden layer. A set of input values represent an input vector. The neurons in a hidden layer receive input from the neurons in the input layer and transmit their output to the neurons in the output layer. The set of output values represent an output vector (Jain, 1994). In such a network, information is propagated in a forward direction from the input to the hidden to the output layers and is thus referred to as feed forward networks. Recall that the error is propagated back from the output to the hidden to the input layer during training (or learning process).

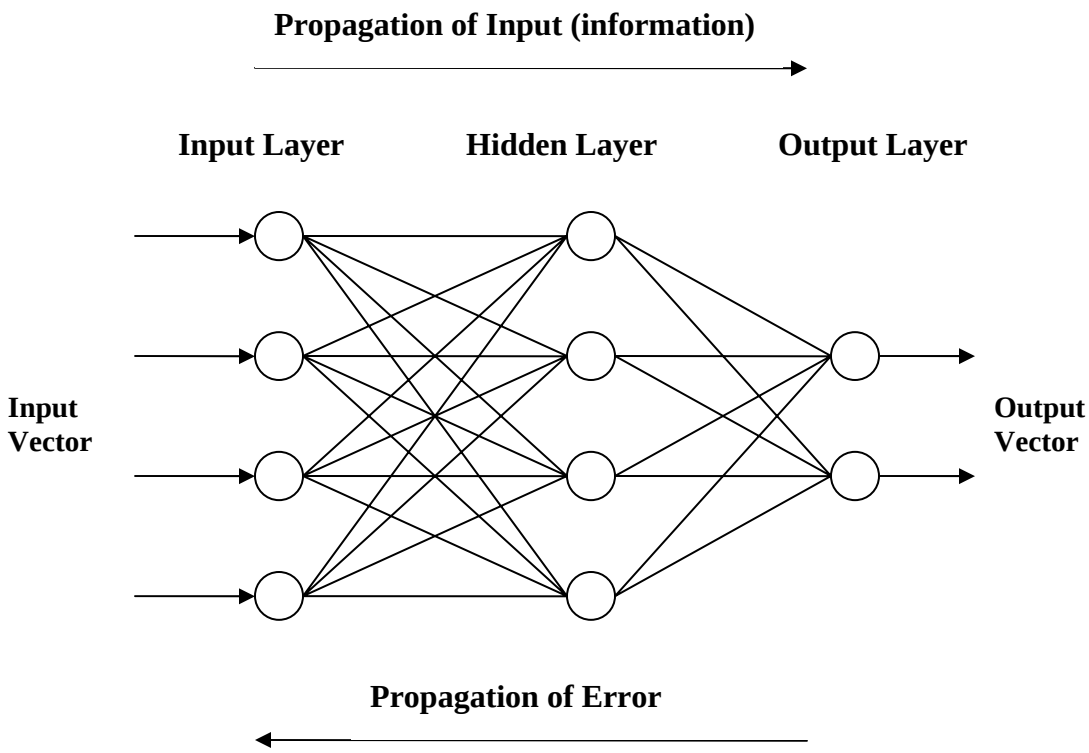


Figure 3-6. Structure of a simple 3-Layer Back Propagation ANN

The activation at a particular neuron is simply the weighted summation of the product of the activation coming from the previous neuron and its associated numeric weight. This is mathematically represented as follows:

$$I_j = \sum_{i=1}^{N_j} w_{ij} O_i \qquad (3\text{-}2)$$

Where,

I_j is the input received by neuron j from neurons in the previous layer,

O_i is the output coming out from neuron i,

W_{ij} is the strength or weight of connection from neuron i to j, and

N_j is the number of neurons in the layer previous to the one in which neuron j is located.

The output from a neuron depends on the transformation function used in the ANN model. The most widely used transformation function is a sigmoid function which is continuous and differentiable (Jain, 1994). The shape of a sigmoid function is shown in Figure 3-7. It has a value between 0 and 1 and can be mathematically described by the following equation.

$$O_j = f(N_j) = \frac{1}{1+e^{-N_j}} \qquad (3\text{-}3)$$

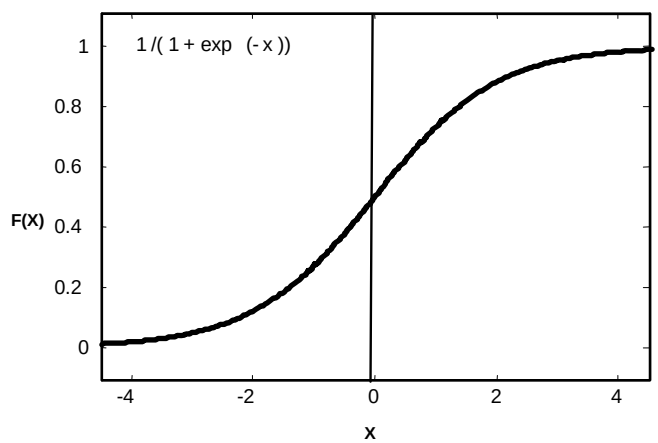


Figure 3-7. The Sigmoid Function

3.5.1.1.4 Training of an ANN

There are two types of training methods in ANNs namely the supervised learning and the unsupervised learning. In supervised learning, the weights that connect the neurons are updated by a mechanism that is controlled externally based on some theoretical concepts. In the case of unsupervised learning, the network itself controls the updating of the weights connecting the neurons based on the kind and behavior of neurons. The most common examples of supervised and unsupervised learning are the back propagation method and self-organizing neural networks respectively (Jain, 1994). For most engineering applications, the back propagation algorithm is commonly used. Muleta (2003) reported that for hydrology-related studies, the back propagation algorithm is a common choice.

3.5.1.1.5 Advantages of ANNs

ANNs have certain advantages over other conventional inductive modeling techniques such as regression and these are summarized as follows:

- In ANN modeling the functional form of the relationship between the input and output variables of the response function being modeled is not required a priori. In fact, a neural network will come up with a relationship based on its learning.
- ANN models can be easily updated with new data.
- ANNs are particularly suited for highly nonlinear and complex response functions for which conventional methods cannot be used. ANNs can work well when the underlying physics of the process modeled is not known.
- ANN models can result in significant reductions in computational time when compared to some of the more complex mechanistic models (Muleta, 2003).

3.5.1.1.6 Limitations of ANNs

ANN models are often referred to as "black box models" as they are not primarily used to produce empirical equation to represent a process, but are rather used to produce outputs according to inputs received by the model. Such models require considerable data for training and are not favorable for applications where the objective is to obtain a simple, easy to use, and functionally compact approximation. As the number of hidden layers and number of neurons in each hidden layer increases, the functional form extracted from these so called black-box models can turn out to be a long expression (a linear and non-linear combination of sigmoidal functions) with numerous terms. Other disadvantages of the ANN-based models as pointed out by Giustolisi and Savic (2004) include parameter estimation and over fitting. Finally, since ANN models are developed without any knowledge of the physics of the process being modeled, it is possible that the resulting model may not be able to establish an effective cause-and-effect relationship between the input and output variables. In such cases, while they serve as good prediction tools of the response function, their use in a management framework requiring a cause-and-effect relationship between variables may be limited.

3.5.1.2 Genetic Programming (GP)

In addition to use in various optimization applications, evolutionary methods have also been successfully used to develop inductive models that fit available data to provide a closed form approximation of the response function. The most successful of these applications have been found in the use of Genetic Programming (GP) which evolves symbolic expressions resulting in a formula for the given data set (Babovic et al., 2001). GP is a branch of genetic algorithms (Koza, 1992). GP can be classified as a machine-learning method that induces a population of computer programs or models that improve automatically as they experience the data on which they are trained (Banzharf et el., 1998). The most frequently used GP method is so-called symbolic regression proposed by Koza (1992) Given a set of variables where some variables are dependent on others, GP helps to develop functions or models that relate the dependent and independent variables. GP evolves tree-like solutions in finding the optimal function (or computer program) that best fits the given data set. Each potential function is evaluated with the given data set and is assigned a fitness value based on how well the model fits into the data set. The main distinctive feature of GP is thus its ability to search for a solution to the given problem by changing model structures (tree-like) rather than by finding better values of model parameters or decision variables. An example tree-representation for the expression X + (Y*Z)) is given in Figure 3-8.

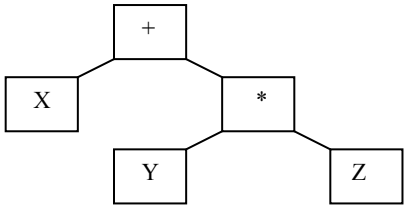


Figure 3-8. Tree-like structure in GP for the expression X + (Y*Z)

These so-called parse trees represent a node-link structure whose nodes are procedures, functions, variables, and constants. In Figure 3-8, the variables X, Y, and Z are leaves in the parse tree and belong to the so-called terminal set, while the mathematical operations + and * are functions and are members of the so-called functional set. Like genetic

algorithms, the genetic operations of crossover and mutation take place in the same manner in GP. Crossover can be achieved by replacing one or more nodes from one individual with those from another, while mutation can be performed by changing a node's argument or operator function. The result of crossover and mutation operations is the production of two new individuals in which they inherit some characteristics of the parents. The process is continued until the fitness of the entire population increases and converges to finding the near optimal solution set. As in most evolutionary algorithms, the models that produce the best fit to the given data set have the greatest opportunity to become parents and produce children. The better models produce the smallest errors, or differences between the calculated output and the observed output. While GP may generate a satisfactory function that reproduces the desires output vector {Y} for a given input vector {X}, there is no guarantee that the resulting model structure obtained by GP will give an insight into the actual working of the system. The general idea of GP can be illustrated as given in Figure 3-9. A training data set is fit to evolving computer programs generated by GP and the resulting optimal program is then used to generate output from given inputs. Application of GP to problems in water resources engineering include Babovic and Keijzer (2000), Davidson et al. (1999), and Babovic and Abbott (1997).

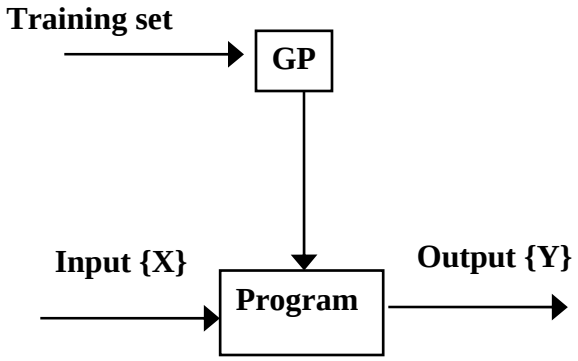


Figure 3-9. General Representation of GP

3.5.1.3 Genetic Functions (GFs)

While GAs have been extensively used for applications in engineering optimization, the methodology has recently been used by several researchers in the development of inductive models. For instance, GAs are traditionally used for finding optimal values of parameters or decision variables of existing models (Alvarez et al, 2000). Chapter 2 describes the in detail the use of GAs as an optimization method. Although similar to GP, GFs employ GAs to build an inductive model from a set of linear and higher order polynomials. Rogers and Hopfinger (1994) and Shi et al. (1998) used GAs to develop inductive models as a combination of linear polynomials as well as polynomials of higher order to represent biological activity using physicochemical properties of a series of compounds. Recently, a new technique called Evolutionary Polynomial Regression (EPR) (Giustolisi and Savic, 2004; Giustolisi et al., 2004) was developed which integrates numerical and symbolic regression to search for an explicit functional approximation of the system being modeled. EPR uses polynomial structures to formulate functional forms and allows a GA search engine to obtain optimal exponents of such expressions (Giustolisi and Savic, 2004; Giustolisi et al., 2004).

More recently, a new evolutionary method based on GAs for functional approximation of response functions from a given data set was introduced by Tufail and Ormsbee (2004). It is referred to as Fixed Functional Set Genetic Algorithm (FFSGA). The method starts with a general pre-defined functional form, and searches for the optimal (best) computer model (empirical expression) by using a GA to search from a fixed set of sub-functions (of independent variables or model inputs) and mathematical operators (Tufail and Ormsbee, 2006). In addition, the structure can include numeric coefficients to provide greater flexibility and accuracy to the resulting model. The basic GA operators used in the search process include the operations of *reproduction, crossover*, and *mutation*. In FFSGA, the user has the ability to control the complexity of the structure by evaluating simple (fewer terms) to complex (greater number of terms) in the formulation. FFSGA also offers the flexibility and diversity to include linear or highly non-linear elementary functions in the library of internal functions provided for the GA search process. Chapter

4 provides a detailed description of this method along with an example application to water resources engineering.

3.5.2 Inductive Watershed Models

Inductive modeling techniques are increasingly becoming popular for the construction of watershed models to model hydrologic and water quality processes. Some of the techniques used for inductive watershed models include artificial neural networks (ANNs) genetic programming (GP), and genetic functions (GFs).

3.5.2.1 ANN-based Inductive Watershed Models

Models based on the principle of ANNs have been considered an alternate to physically based models, due to their simplicity relative to minimizing the need for collecting detailed watershed data. ANN modeling methodology offers a promising alternative to the traditional time-series approach for developing input-output simulations, and to the use of hydrologic models that require modeling the internal processes of a watershed (Zealand et al. 1999). In the context of watershed modeling, current research on ANN-hydrologic applications ranges from the predictions of peak discharge and time to peak from a single rainfall event, to the forecast of hourly or daily river stages or discharges (Wu et al. 2005). Zealand et al. (1999) and Wu et al. (2005) provide listings of significant contributions related to the use of ANNs for hydrological modeling. Recently, Muleta (2003) developed an ANN model to mimic SWAT (U.S. Department of Agriculture Soil and Water Assessment Tool) outputs and used the resulting inductive model in an optimal management model for controlling non-point source pollution.

Recently there are successful applications of ANN in biological/pathogens modeling and identification of pollution sources. These include Lingireddy and Brion (2004), Brion *et. al*. (2004), Brion and Lingireddy (2003), Neelakantan *et al*. (2002), Brion *et al*. (2002), Neelakantan *et al*. (2001), Brion and Lingireddy (2000), Brion and Lingireddy (1999), Brion et al. (2001), and Suen and Eheart (2003). Tufail and Ormsbee (2005b) recently

developed an ANN-based inductive receiving water model for Beargrass Creek watershed in Louisville, Kentucky for predicting nutrient loads (total phosphorus and total nitrogen) and dissolved oxygen concentrations in the receiving streams. Tufail and Ormsbee (2005c) have also developed an ANN-based inductive model for predicting the monthly geometric mean of fecal coliform in surface water bodies. Both of these later applications will be discussed in more detail in Chapter 5.

3.5.2.2 GP-based Inductive Watershed Models

Babovic (1996) first introduced the idea of GP in the area of water resources and since then a number of researchers have used the technique to analyze water management problems. Application of GP to rainfall-runoff problems can be found in Drecourt (1999) and Savic et al. (1999). Drunpob et al. (2005) developed a GP model to forecast stream flow rates in a semi-arid coastal watershed. More recently, Jayawardena et al. (2006) performed a comparative analysis of a data driven model based on GP with GIS-based conceptual rainfall-runoff model and demonstrated the potential of GP as a viable data-driven rainfall-runoff model.

3.5.2.3 GF-based Inductive Watershed Models

GF-based inductive watershed models are based on the recently developed GA-based method of functional approximation called FFSGA (fixed functional set genetic algorithm). These include the development of a FFSGA-based inductive model (Tufail and Ormsbee, 2005b) for the three forks of Beargrass Creek watershed in Louisville, Kentucky for predicting nutrient loads, and the development of an inductive model for predicting the monthly geometric mean of fecal coliform in surface water bodies (Tufail and Ormsbee, 2005c). The FFSGA technique is discussed in detail in Chapter 4. FFSGA-based inductive models for nutrients and pathogens are discussed in Chapter 5.

CHAPTER 4
A FIXED FUNCTIONAL SET GENETIC ALGORITHM (FFSGA) APPROACH TO INDUCTIVE MODELING

4.1 Introduction

The goal in most modeling is to find an optimal balance between model complexity and model applicability by applying basic principles of model parsimony. The principle of parsimony states that we employ the smallest possible number of parameters in a model (Box and Jenkins, 1976). Process-based or deductive models can be often comprised of too many parameters that need to be calibrated and can lead to computational expense and added complexity. Inductive or data-driven models are becoming more and more popular due to their ease of use and simplicity as substitutes for more complex process-based models in a number of applications. For instance, inductive models may be preferred where 1) computational expense is a critical issue, 2) the process-based deductive model is over parameterized and cannot be adequately calibrated, and 3) budgetary constraints do not allow for a complex deductive model. More recently, inductive models derived using evolutionary and biological principles are becoming increasingly popular. Chapter 3 provided a description of several of such inductive modeling techniques including artificial neural networks (ANN) and genetic programming (GP). Both ANN and GP have been successfully used to develop inductive models for applications in water resources engineering. In cases where a simple and compact empirical relationship is sought for the response function being modeled, a new technique called FFSGA (fixed functional set genetic algorithm) is proposed (Tufail and Ormsbee, 2006).

While GP has been successfully used in model building of response functions, they often result in complex expressions for the function sought that are not often simple and easy to use. Also, such expressions can be difficult to interpret and could lead to over fitting of the problem (Giustolisi and Savic, 2004). The fact that empirical models resulting from GP are of variable size and shape as model structures continuously undergo adaptations

from a class of parse trees explains variability in the resulting optimal model. An example of this can be seen in the explicit polynomial approximation model for friction factor in turbulent pipe flow using GP in the work done by Davidson et al (1999).

ANN-based inductive models require considerable data for training and are not favorable for applications where the objective is to obtain a simple, easy to use, and functionally compact approximation. As the number of hidden layers and number of neurons in each hidden layer increases, the functional form extracted from these black-box models can turn out to be a long expression (a linear and non-linear combination of sigmoidal functions) with numerous terms. Other disadvantages of the ANN-based models as pointed out by Giustolisi and Savic (2004) include parameter estimation and over fitting.

More recently, a new technique called Evolutionary Polynomial Regression (EPR) was developed which integrates numerical and symbolic regression to search for an explicit functional approximation of the system being modeled (Giustolisi and Savic, 2004, Giustolisi et al., 2004). The disadvantages of GP and ANN mentioned above were some of the key motivators for this new GA-based polynomial functional approximation. EPR uses polynomial structures to formulate functional forms and allows a GA search engine to obtain optimal exponents of such expressions. The proposed FFSGA method of inductive model building is also derived from a motivation to develop data-based inductive models that are simple to implement and produces compact and easy to use explicit expressions. FFSGA is different from EPR (Giustolisi and Savic, 2004) in that it does not use a polynomial structure for functional approximation, and allows the user to formulate any pre-defined form comprised of functions of model inputs (or combination of such functions), coefficients, and operators.

4.2 Fixed Functional Set Genetic Algorithm (FFSGA)

An inductive model represents a relationship between independent variables (model inputs) and a target response function (model output) that is being modeled. In the proposed FFSGA method, a pre-defined general functional form is formulated

comprising of coefficients, sub-functions of independent variables or model inputs, and mathematical operators. A GA algorithm is then used to search for the best combination of sub-functions of the model inputs (logarithmic, exponential, sine, cosine, etc.) and mathematical operators (+, -, *, /, ^) that will fit the pre-defined functional form while minimizing the difference between observed and predicted outputs. The coefficients in the pre-defined functional expression are then sought using least squares optimization by starting from a pre-evolved starting point. The library of sub-functions of the independent variables is provided by the user. As would be expected, a library with greater number of sub-functions will ensure more choices for the GA search process leading to better functional approximation results. Such a method is particularly suited for applications where some relationships between the input and output variables may be known or at least hypothesized (e.g., logarithmic or exponential relationship). The distinct feature of this method that distinguishes it from a standard GP-based inductive modeling technique is that the general form of the approximation function sought is defined prior to the evolutionary search process. However, in the absence of prior knowledge about the response function sought, it is still possible with considerable ease to formulate "a very general" form via some logical arrangement of coefficients, functions of independent variables (model inputs), and mathematical operators. Such a starting formulation determines the number of parameters and elementary functions to be used in the functional form sought and thus allow the user to control the complexity of the expression. The most optimal expression at the end of the search process becomes the functional approximation of the response function under study.

The process of obtaining the optimal functional form using FFSGA is thus achieved in two steps. In the first step, the GA searches for the optimal functions of the decision variables and mathematical operators to obtain the optimal functional components that will constitute the structure of the desired functional form. In the second step, the coefficients of the functional form are obtained by least squares optimization. Such an approach helps in eliminating any potential convergence problems associated with searching for numeric coefficients (constants) and functional forms (sub-functions of independent variables and mathematical operators) at the same time. By searching for

the numeric coefficients and functional forms (sub-functions of independent variables and mathematical operators) at the same time can lead to convergence problems thus restricting the ability of FFSGA to be effective in obtaining optimal expressions.

FFSGA is static in the sense that the general shape and size of the pre-defined functional form does not change during the GA search. The pre-defined functional form can be based on any prior knowledge of the response function or the user can formulate several general formulations without any such knowledge. The pre-defined formulations can be varied by varying the structure and corresponding number of terms (parameters) in the functional form as deemed appropriate by the user. This is different from the GP approach in which the parse tree structures (that represent the functional form) are dynamic and change form as they evolve to obtain the most fit functional form or expression for the data set being analyzed. This static GA approach results in the optimal selection of a functional form or expression that can be simple, easy to use, and compact after training on a given data set. The method uses the basic structure of GA optimization involving selection, crossover, and mutation processes by selecting sub-functions of independent variables (model inputs) and mathematical operators that minimizes the mean square error between the observed and predicted output.

4.3 FFSGA Methodology

FFSGA is a GA-based method to develop inductive models for a response function sought. For a given function Y for which an empirical functional form is sought, a pre-defined functional form(s) is first selected. Such a formulation can be based on any prior knowledge about Y or can be formulated without such knowledge. The pre-defined functional form is a function of the independent variables (say X1 and X2) and one such formulation is given in Figure 4-1.

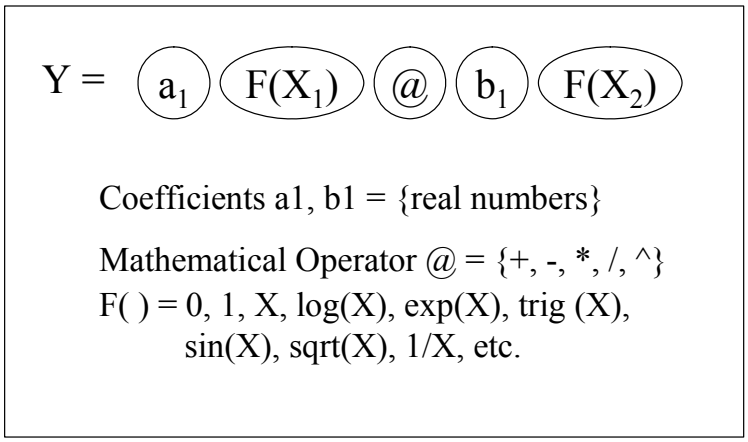


Figure 4-1. General pre-defined functional form for response function Y

The objective function in the search process is the explicit functional form sought (Figure 4-1) for Y (model output) and the fitness function is based on the mean square error (MSE) of the performance of the objective function in predicting the value of Y as a function of the two decision variables X1 and X2 (model inputs). More than one functional form can be formulated for Y by varying the parameters and functional structure of the function sought. Also, the user can increase the number of available sub-functions of the independent variables for selection in the GA process.

The basic genetic operations of GA (selection, crossover, and mutation) are used to select the best sub-functions and operators as identified in the pre-defined functional form given in Figure 4-1. The FFSGA model starts with a random selection of solution sets resulting in an initial population. Each solution set thus represents an explicit equation for the target variable Y. GA works on a population of possible solutions attempting to find the optimal solution (in this case the most fit computer program or functional form) that maximizes the value of the fitness function. In each generation, some population of solutions improves the fitness function and others get worse. The superior solutions are used in producing the next generation of populations to continue the search process. The FFSGA model continues to evolve a new set of solution vectors as the search marches from one generation to the other. It is possible that some of the individuals (off-springs) may be worse than their parents as the average fitness of solutions generally increases.

The improved solution sets tend to survive from generation to generation, and those that are inferior (poor fitness values) will tend to die out in the process. At the termination of the specified number of generations, the functional form that has the highest fitness value is selected as the optimal structure of the explicit expression sought in the search process. Finally, the coefficients of the functional form are obtained by applying least squares optimization to the optimal form obtained from the GA process. The FFSGA approach works in a manner similar to GP, except that the general functional form is pre-defined and it does not change size and form. The FFSGA approach can be illustrated by the flow chart as shown in Figure 4-2.

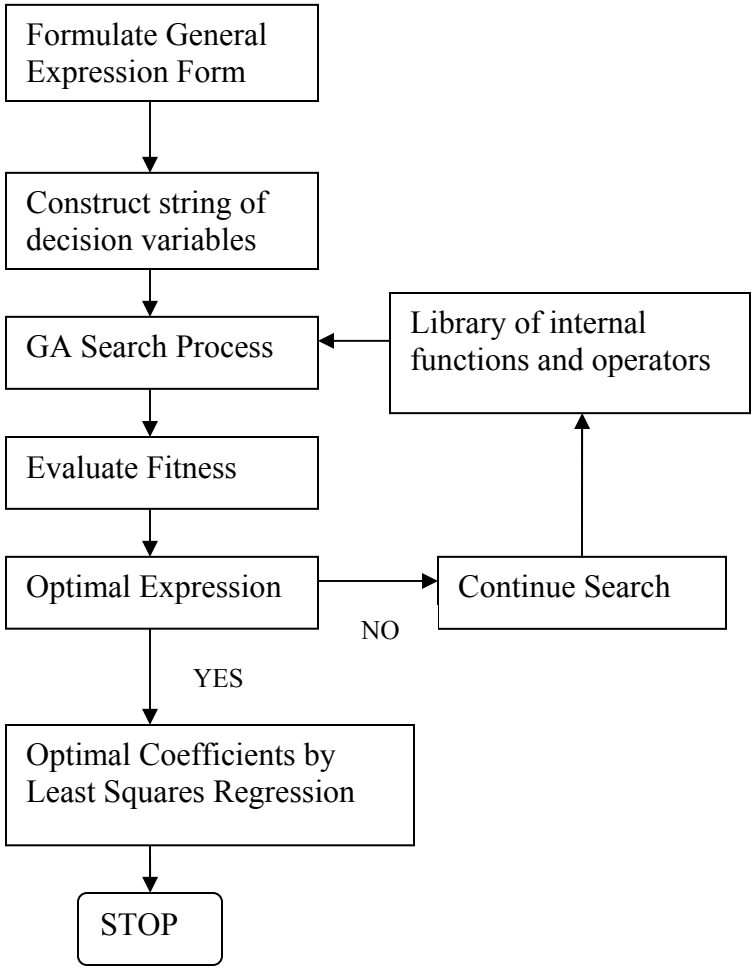


Figure 4-2. Flow Chart of FFSGA Model

4.4 FFSGA Search Strategy

FFSGA is a general methodology that can be applied to obtain functional approximation of a response function under study. The open-ended nature of the technique that allows the user to evaluate any desired form and associated sub-functions (linear and/or non-linear) is strength of this approach that can bring more flexibility and diversity to the search process. The following guidelines will aid the user to specify a starting pre-defined formulation and associated library of internal functions (of model inputs) for the GA search process:

1. Given the number of independent variables (model inputs), the starting functional form (e.g. as given in Figure 4-1) can include any number of coefficients, sub-functions of model inputs, and mathematical operators as desired by the user. The user can control the complexity of the form in this stage and it is recommended to start from a simple form (fewer terms) and move to more complex forms by adding more terms.

2. Given a starting functional form, the GA would need a library of sub-functions of the independent variables (model inputs) to search for the most optimal sub-functions. A breadth first and depth next approach of elementary sub-function search is suggested here. For any given functional approximation sought, the user can start with a limited set of generally perceivable sub-functions of the model inputs (such as logarithmic, exponential, sine, square root, etc.) as well as combination of such sub-functions. The FFSGA model can be run with this initial library of sub-functions to evaluate the goodness of fit obtained for the response function. Based on the results of the model application, if the resulting expression is within the model performance criteria, the user can 1) stop, or 2) further improve model performance by focusing on the optimal function types selected by the GA search and introducing more variations of that particular function type in the library of sub-functions.

3. If the model performance with the initial library of sub-functions is not within a prescribed target (such as a target MSE value), the user can continue to add more elementary sub-functions or combination of sub-functions to the library of sub-functions to provide more flexibility and diversity to the search process. The process continues until a functional expression is obtained that satisfies the user's performance criteria. It should be noted that any prior knowledge of the response function will obviously facilitate the search process as it allows the user to select functions (and its variations) that can better describe the process.

4.5 Example Application (Friction factor for flow in pipes)

The proposed fixed functional set genetic algorithm (FFSGA) approach will be used to derive a function to represent the relationship between friction (*f*) and the three independent variables of pipe diameter (*D*), pipe roughness (*E*), and the Reynolds number (*Re*). The resulting closed form expression(s) for the friction factor will be compared with an explicit polynomial expression derived previously by Davidson et al. (1999) using GP coupled with polynomial regression. The resulting closed form expression(s) will also be compared to an explicit expression for friction factor, known as the Swamee and Jain equation (Swamee and Jain, 1976).

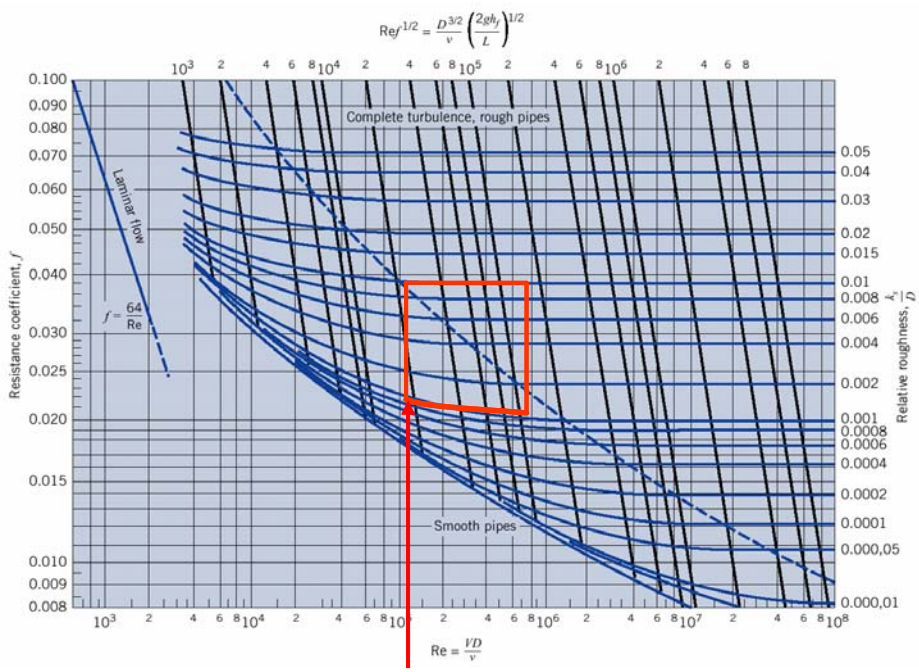
The calculation of energy (or head) loss in pipe flow is the one of the most frequently calculated quantities in the area of fluid mechanics. For a given pipe with diameter D, the head loss can be calculated using the Darcy-Weisbach equation as follows (Potter and Wiggert, 1991):

$$H_L = \frac{f L V^2}{2 g D} \qquad (4\text{-}1)$$

Where, H_L is the head loss in pipe, *f* is the friction factor, *V* is the velocity, *D* is the pipe diameter, and *g* is the gravitational constant. The friction factor *f* depends on the relative roughness of the pipe (*E/D*) and pipe velocity (through Reynolds Number $Re \equiv VD/\upsilon$),

and is computed either by implicit or explicit equations available or a chart-based solution such as Moody diagram (Moody, 1944) is used. Experimental data that relate the friction factor f to the Reynolds number Re have been developed for fully developed pipe flow over a wide range of wall roughness (Potter and Wiggert, 1991). The results of these data are available in the form of what is commonly referred to as the Moody Diagram (Figure 4-3) as given in most fluid mechanics books (Moody, 1944). In practice, most of the pipe flow calculations lie in the turbulent zone ($4000<Re<10^8$). Empirical equations exist that represent the turbulent zone of the Moody Diagram (Moody, 1944). Two of the most frequently used equations are presented here and these include the Colebrook-White equation (Colebrook, 1939) and the Swamee and Jain equation (Swamee and Jain, 1976). For turbulent pipe flow, the Moody diagram (Moody, 1944) is a graphical representation of the Colebrook-White equation as given in Equation (4-2).

$$\frac{1}{\sqrt{f}} = -0.86 \ln\left(\frac{E}{3.7D} + \frac{2.51}{\mathrm{Re}\sqrt{f}}\right) \qquad (4\text{-}2)$$



Transitional zone region used in the example application

Figure 4-3. Moody's Diagram (Moody, 1944)

The most significant drawback of using Equation (4-2) is its implicit nature, i.e., the friction factor *f* appears on both sides of the equation, thus requiring the use of iterative methods to solve for *f*. Regardless of this drawback, the Colebrook-White equation is considered the most accurate formula to compute friction factor *f* for pipe flow computations in the turbulent zone. The Swamee and Jain (Swamee and Jain, 1976) equation is an explicit equation for obtaining the friction factor *f*, and for turbulent flow regime is given as follows:

$$f = \frac{0.25}{\left(\log_{10}\left(\frac{E}{3.7D} + \frac{5.74}{\mathrm{Re}^{0.9}}\right)\right)^2} \qquad (4\text{-}3)$$

$$10^{-6} < E/D < .01 \text{ and } 5000 < \text{Reynolds Number} < 3\text{x}10^{8}$$

The Swamee and Jain (Swamee and Jain, 1976) equation is accurate to within approximately 2% of the Moody diagram (Moody, 1944).

The purpose of this example application is to find an explicit functional approximation for the friction factor *f* for turbulent pipe flow as a function of *Re* (Reynolds number) and *E/D* (relative roughness of the pipe material) for a specific region in the transitional zone of Moody Diagram. This region lies between Reynolds numbers ranging from 100,000 to 1,000,000 and relative roughness values from 0.001 to 0.01 as highlighted in Figure 4-3. For the purpose of this study, the Colebrook-White equation was used to generate a data set consisting of a two-dimensional grid of 100 data points, created from 10 Reynolds values selected in equal increments of 100,000 on the interval of 100,000 to 1,000,000, and 10 relative roughness values selected in equal increments of 0.001 on the interval of 0.001 to 0.01. Davidson et al. (1999) used the same data set for finding an explicit polynomial function for friction factor *f* using GP. The performance of the explicit functional form using FFSGA is compared to the Swamee and Jain equation (Swamee and Jain, 1976) and the results obtained by Davidson et al. (1999).

4.5.1 FFSGA Methodology for Friction Factor Functional Form

The objective function in the example application is the explicit functional form sought for the friction factor and the fitness function is based on the mean square error (MSE) of the performance of the objective function in predicting the friction factor as a function of the two independent variables (model inputs). These two independent variables include the relative roughness of the pipe (E/D) and Reynolds number (Re). Note that E is defined as the average height of surface irregularities of the pipe and D is the pipe diameter. These are the same variables that are plotted on Moody Diagram (Figure 4-3) in determining the friction factor for turbulent pipe flow. Five general functional forms were formulated to represent the expression for friction factor in the transitional flow zone. Each of these forms is comprised of some logical combination of the two independent variables (or sub-functions of the two independent variables), some numeric coefficients, and mathematical operators, and are given in Figure 4-4. It should be noted these functional forms were formulated in a general way so as not to mimic or replicate any particular functional form such as the Swamee and Jain equation (Swamee and Jain, 1976). In other words, these general functional forms were formulated without any attempt to match an already existing explicit form. However, in a typical application, prior knowledge of the functional form can be used to develop such formulations thereby facilitating the search process. The user can formulate and evaluate any number of such functional forms for the response function being modeled, and the five given in Figure 4-4 are formulated here for the sake of demonstration. Table 4-1 gives a list of a sample of 15 different internal or elementary sub-functions for the two independent variables (model inputs) that are available for selection by the FFSGA model. The number of such elementary sub-functions can be expanded further by introducing more sub-functions or combination of sub-functions. Table 4-2 gives the corresponding mathematical operators that are available for selection by the FFSGA model.

Functional Form #1 = {C_1 operator_1 [function_1 (E/D) operator_2 function_2 (Re)]} operator_3 {C_2 operator_4 [function_3 (E/D) operator_5 function_4 (Re)]}

Functional Form #2 = {C_1 * [function_1 (E/D) operator_1 function_2 (Re)]} operator_2 {C_2 * [function_3 (E/D) operator_4 function_4 (Re)]}

Functional Form #3 = {C_1 * function_1 (E/D) * function_2 (Re)} operator_1 {C_2 * function_3 (E/D) * function_4 (Re)}

Functional Form #4 = {C_1 * function_1 (E/D)} operator_1 {C_2 * function_2 (Re)}

Functional Form #5 = {[C_1 * function_1 (E/D)] operator_1 [C_2 * function_2 (Re)]} operator_2 {C_3 * function_3 (E/D) * function_4 (Re)}

Figure 4-4. Pre-defined Functional Forms

As seen in Figure 4-4, all of the five functional formulations are defined in terms of some function of the independent variables. For example, "function_1 (E/D)" in functional form #1 can be selected to be any of the 15 sub-functions defined in Table 4-1, and so on. Similarly, "operator_1" in functional form #1 can take on any of the five operator values given in Table 4-2. The coefficients C_1, C_2, and C_3 are double precision real numbers.

Table 4-1. List of functions for Decision Variables (Re and E/D)

Function #	Function f (Re) or Function f (E/D)
1	1
2	Re or E/D
3	1/Re or 1/(E/D)
4	Exp (Re) or Exp (E/D)
5	Log_e (Re) or Log_e (E/D)
6	Log_{10} (Re) or Log_{10} (E/D)
7	Exp (1/Re) or Exp (1/(E/D))
8	Log_e (1/Re) or Log_e (1/(E/D))
9	Log_{10} (1/Re) or Log_{10} (1/(E/D))
10	Re*Exp (Re) or (E/D)*Exp (E/D)
11	Re* Log_e (Re) or (E/D)*Log_e (E/D)
12	Re*Log_{10} (Re) or (E/D)*Log_{10} (E/D)
13	1/Re*Exp (Re) or 1/(E/D)*Exp (E/D)
14	1/Re* Log_e (Re) or 1/(E/D)*Log_e (E/D)
15	1/Re*Log_{10} (Re) or 1/(E/D)*Log_{10} (E/D)

Table 4-2. List of Mathematical Operators

Operator #	Operator
1	+
2	-
3	*
4	/
5	^

The basic genetic operations of GA are used to select the optimal elementary sub-functions (from Table 4-1) and operators (from Table 4-2) for inclusion in the each of the five pre-defined functional forms given in Figure 4-4. Each individual solution set in the GA process consists of a chromosome of decision vectors that makes up the structural components (sub-functions and operators) of the general functional form sought as given in Figure 4-4. Thus the length of the solution set (chromosome) for each of the five functional forms given in Figure 4-4 will vary according to the number of terms. These chromosomes are represented as strings of values in binary form (0 or 1). For example, in the case of functional form #1 (Figure 4-4), there are 9 decision vectors in each solution set (chromosome). These are given as follows:

<u>Solution set</u> operator_1, operator_2, operator_3, operator_4, operator_5, function_1, function_2, function_3, and function_4

Note that the coefficients in functional form #1 are not sought in the GA search process and thus are not included in the solution set (chromosome). In the FFSGA model, strings of binary numbers of fixed length represent the values of the decision vectors contained in the solution set given above. The length of each string representation depends on the numeric bounds of the individual parameter being represented. For example, since operator_1 through operator_5 can have a value between 1 and 5 as given in Table 4-2, they can be represented by a 3-digit binary string. Note that the maximum decimal value of a 3-digit binary string is 7, and appropriate mapping is performed in the decoding of binary numbers. Similarly, if function_1 through function_4 can have a value between 1 and 15 as given in Table 4-1, each of these sub-functions can be represented by a 4-digit

binary string. Note that the maximum decimal value of a 4-digit binary string is 15. Consequently, for functional form #1, the total length of each solution set (chromosome) will be 31 for this particular illustration and is represented as follow (Table 4-3):

Table 4-3. Allocation of binary strings to decision vectors in a solution set (chromosome) for Functional Form #1

String	**Operator_1**	**Operator_2**	**Operator_3**	**Operator_4**	**Operator_5**
# of binary digits	3	3	3	3	3
String	**Function_1**	**Function_2**	**Function_3**	**Function_4**	
# of binary digits	4	4	4	4	

4.5.2 FFSGA Results for Friction Factor

The FFSGA model evaluates each of the five functional forms (Figure 4-4) individually. In other words, a separate search is conducted for each of the five formulations. In each case, the model starts with a random selection of solution sets resulting in an initial population. Each solution set thus represents an explicit equation for the friction factor. These solution sets are evaluated for the given data set (values of Re and E/D in this case) and the computed values of friction factor are compared against the target or actual function values to determine the mean square error (MSE). The MSE is a measure of how good the given solution set is in representing the data set evaluated and translates into the corresponding fitness function. The FFSGA model continues to evolve new set of solution vectors as the search marches from one generation to the other. This is accomplished through the process of selection of new generation populations, crossover, and mutation. Each functional form is evaluated individually by varying the number of populations, generations, and the probability of crossover and mutation in the GA search process. The results of the analysis reveal that the GA search process produces the optimal expressions when the probability of crossover and mutation is fixed at 0.7 and 0.03 respectively. At the termination of specified generations, the functional form that has the highest fitness value is the optimal structure of the explicit expression sought in the search process. Finally, the coefficients of the functional form are obtained by applying least squares optimization to the optimal form obtained from the GA process.

The final expressions representing the optimal functional forms for each of the five general forms are given below (Equations 4-4 through 4-8). Table 4-4 gives the corresponding MSE values and maximum error of interpolation for the data set analyzed by each of the optimal expressions namely FFSGA-Function 1 through 5. It is evident from the results that the FFSGA approach produces several compact and easy to use expressions for obtaining the friction factor *f* for a given data set consisting of *Re* and *E/D* values in the transitional zone. Also given in Table 4-4 are the MSE values for the same data set for the expressions resulting from the GP approach used by Davidson et al. (1999) as well as the Swamee and Jain equation (Swamee and Jain, 1976).

$$f = \frac{-32.48 - \left[\left(\frac{1}{E/D}\right) * \exp(E/D) - \log_{10}(\mathrm{Re})\right]}{16.14 * \left[\left(\frac{1}{E/D}\right) * \log_{10}(E/D) + \log_{10}\left(\frac{1}{\mathrm{Re}}\right)\right]} \tag{4-4}$$

$$f = \frac{10.84 * \left[(\exp(E/D)) \wedge \log_{10}(\mathrm{Re})\right]}{84.69 * \left[\ln(E/D) - 1\right]} \tag{4-5}$$

$$f = \frac{\left[11.71 * (\exp(E/D)) * \mathrm{Re} * \log_{10}(\mathrm{Re})\right]}{\left[71.71 * \left(\log_{10}\left(\frac{1}{E/D}\right)\right) * \mathrm{Re} * \ln(\mathrm{Re})\right]} \tag{4-6}$$

$$f = \left[4.161 * \log_{10}\left(\frac{1}{E/D}\right)\right]^{\left[-1.543 * \exp\left(\frac{1}{\mathrm{Re}}\right)\right]} \tag{4-7}$$

$$f = \frac{\left[3.60 * (E/D) * \exp(E/D)\right] + \left[-0.027 * \log_{10}\left(\frac{1}{\mathrm{Re}}\right)\right]}{-0.082 * \left[\ln(E/D) * \ln(\mathrm{Re})\right]} \tag{4-8}$$

Table 4-4. MSE and Maximum Error values for example application (Data set from Moody Diagram)

Expression Type/Method	MSE	Max. Absolute Error
FFSGA-Function 1 (Equation 4-4)	0.00000020	0.001229585
FFSGA-Function 2 (Equation 4-5)	0.00000050	0.001848040
FFSGA-Function 3 (Equation 4-6)	0.00000315	0.003719280
FFSGA-Function 4 (Equation 4-7)	0.00000011	0.001807310
FFSGA-Function 5 (Equation 4-8)	0.00000022	0.001281080
2-term GP term by Davidson et al (1999)	0.00000082	0.002293470
4-term GP term by Davidson et al (1999)	0.00000016	0.001499050
5-term GP term by Davidson et al (1999)	0.00000009	0.001491670
10-term GP term by Davidson et al (1999)	0.00000002	0.000693730
14-term GP term by Davidson et al (1999)	0.000000002	0.000193930
Jane and Swamee Equation	0.00000002	0.000253750

It can be seen in the Table above that the expressions resulting from the FFSGA approach competes well with all other methods. Of the five pre-defined functional forms evaluated, the best results are obtained by using the FFSGA-Function 4 as given by Equation (4-7), and even though it does not compete with some of the higher order polynomial expressions derived by Davidson et al. (1999) in terms of accuracy, the expression is simple, compact, and easy to use. The 14-point expression derived by Davidson et al (1999) as given in Equation (4-9) may be of greater accuracy (MSE is superior to the most accurate FFSGA expression by two significant digits), but results in an expression that is not as compact and simple as the ones derived by the FFSGA model.

$$\begin{aligned} y \;=\; & 1.222995307(10^{-5})X_1^{\,6}X_2^{\,5} - 2.242748136(10^{-10})X_1^{\,5}X_2^{\,5} - 2.482162347(10^{-4})X_1^{\,5} \\ & + 9.286977109(10^{-6})X_1^{\,3} + 3.645038671(10^{-2})X_1^{\,3} - 1.18044694(10^{-3})X_1^{\,2}X_2^{\,2} - \\ & 0.3849323423\,X_1^{\,2} + 6.598401765(10^{-2})X_1X_2 + 2.522401137X_1 + \\ & 6.471827292(10^{-4})X_2^{\,4} - 1.77688826(10^{-2})\,X_2^{\,3} + 0.1829816121X_2^{\,2} - \\ & 0.9369530943X_2 - \;\; 0.3698214152 \end{aligned} \tag{4-9}$$

Where

$$X1 \;=\; 1000 * \frac{E}{D} \tag{4-10}$$

$$X_2 = \frac{\mathrm{Re}}{100,000} \tag{4-11}$$

$$y = 10 * \frac{f - 0.0199435}{0.0385035 - 0.0199435} \tag{4-12}$$

It should also be noted that in the GP approach used by Davidson et al. (1999) to derive expressions for friction factor, the independent variables (*Re* and *E/D*) and target value (*f*) were transformed to fit on a scale ranging from 1 to 10. This was done to reduce ill-conditioning in the computations. Thus the resulting expressions are in terms of a transformed friction factor (denoted as y in the Equation 4-12), which would need to be converted back into the actual friction factor using the transformation function. In contrast, FFSGA approach uses the actual data set and no transformation is performed thus resulting in computational savings.

4.6 Sensitivity Analysis

In the FFSGA example application described above, none of the five general pre-defined functional forms given in Figure 4-4 are structured to replicate the Swamee and Jain equation with regard to the sub-functions of independent variables, operators, and coefficients. For instance, none of the sub-functions given in Table 4-1 include functions that are dependent on both *Re* and *E/D*. In fact, all of them are either a function of *Re* or *E/D*. A sensitivity analysis was performed to evaluate the performance of the proposed technique by formulating a new functional form #6 (in addition to the five given in Figure 4-4) that in some way replicates the structure of the Swamee and Jain equation. This is done by introducing functions that are dependent both on *Re* and *E/D*. This functional form #6 is given by Equation (4-13) as follows:

$$f = \frac{C_1 * \left(function\left(C_2 * \frac{E}{D} \quad OPER(+-*/) \quad C_3 * \mathrm{Re} \right) \right)^{C_4}}{C_5 * \left(function\left(C_6 * \frac{E}{D} \quad OPER(+-*/) \quad C_7 * \mathrm{Re} \right) \right)^{C_8}} \tag{4-13}$$

The FFSGA model when applied to such a starting functional formulation then finds the optimal sub-functions and operators by a GA search as described previously. The optimal coefficients C_1 through C_8 are obtained by least squares optimization. The optimal expression obtained by using Equation (4-13) as the starting functional form is given by Equation (4-14) and its performance matches that of the Swamee and Jain equation (MSE = 0.00000002) and is given below:

$$f = \frac{0.267}{\left(\log_{10}\left(0.222*(E/D) + \frac{6.69}{\mathrm{Re}}\right)\right)^2} \qquad (4\text{-}14)$$

FFSGA-Function 6 given by Equation (4-14) is also similar in performance to the 10-term expression by Davidson et al (1999). Table 4-5 gives a comparison of the performance of this improved FFSGA expression and those derived by Davidson et al. (1999) as well as the Swamee and Jain equation (Swamee and Jain, 1976). The ability of the FFSGA model to match the performance of the explicit Swamee and Jain equation given a starting functional form (Equation 4-13) that benefits from prior knowledge of the response function highlights two things; 1) FFSGA improves in performance when some knowledge of the response function is known, and 2) FFSGA produces an optimal expression that looks similar to the Swamee and Jain equation. The improved performance validates the promise that this approach has shown in functional approximation of response functions. This sensitivity analysis was carried out to show that prior knowledge about the response function will benefit the FFSGA approach by facilitating the search process and achieving better accuracy. It should however be noted that the GA may return other optimal expressions with different sub-functions that may provide the same accuracy. This is anticipated as the search process is driven by the fitness of the expressions and there may be other sub-functions or combinations of sub-functions and corresponding coefficients that would result in expressions of comparable accuracy. It is however worth noting that given the limited number of sub-functions of the independent variables (initial library of function provided in Table 4-1) available for selection by the FFSGA model and the fact that all starting functional forms (Figure 4-4)

were formulated without prior knowledge of the response function, the performance of the FFSGA-based expressions (Equations 4-4 through 4-8) is quite encouraging. It can thus be anticipated that expanding the library of sub-functions and/or combination of sub-functions will bring more variability to the FFSGA model, and it can be expected to further improve its performance, ultimately approaching that of the Colebrook-White equation. Such an expansion can be carried out either by conducting a breadth first and depth next search for optimal sub-functions or with the help of any knowledge that the user might have about the response function.

Table 4-5. Optimal FFSGA Results
(MSE and Maximum Error values for example application)

Expression Type/Method	MSE	Max. Absolute Error
FFSGA-Function 6 (Equation 3-10)	0.000000020	0.000883490
2-term GP term by Davidson et al (1999)	0.000000820	0.002293470
4-term GP term by Davidson et al (1999)	0.000000160	0.001499050
5-term GP term by Davidson et al (1999)	0.000000090	0.001491670
10-term GP term by Davidson et al (1999)	0.000000020	0.000693730
14-term GP term by Davidson et al (1999)	0.000000002	0.000193930
Jane and Swamee Equation	0.000000020	0.000253750

4.7 General Remarks

The use of inductive models that replicate existing deductive models is gaining popularity and this method provides a simple and useful tool for developing explicit relationships for a response function. This method serves as a useful candidate for application in areas such as:

- Rainfall-runoff modeling
- Watershed response models such as pathogen and nutrient load models (Tufail and Ormsbee, 2005c) and
- Receiving water models such dissolved oxygen models (Tufail and Ormsbee, 2005b).

The fact that FFSGA results in simple and compact expressions for a response function being modeled makes it an ideal candidate for use as a simulation model for integration into an optimization framework. Such integration can be quite cumbersome and computationally expensive if more complex deductive models are to be used. An added benefit of the approach is that it allows the user to control the complexity of the functional form sought by incorporating fewer or more terms in the starting functional formulation. FFSGA also offers the flexibility and diversity to include linear or highly non-linear elementary functions in the library of internal functions provided for the GA search process. Other methods such as GP may be able to develop more accurate expressions, but it may be at the expense of increasing complexity in the form and size of such expressions (as demonstrated in the case of GP-based expressions by Davidson et al. (1999). While the fixed functional framework of the proposed technique may limit the accuracy of the resulting models, such a compromise may be offset by a final model that is simple, compact, and easy to use (Tufail and Ormsbee, 2006). A limitation of the proposed method is the selection of pre-defined general functional forms for the response function. However, the fact that one can formulate such general forms without requiring any prior knowledge of the functional form sought still makes it an effective technique.

Another limitation of the proposed FFSGA methodology for developing inductive models is its ability to handle a large number of inputs in the model. Being in the early development stage, the method is currently well suited and tested on problems involving a manageable number of model inputs (up to 5). As the number of inputs increase, the pre-defined functional form formulated by the user as required can become complex. A methodology to handle large number of model inputs is needed to facilitate the search process while maintaining a compact and easy to use empirical structure of the model sought. Work is underway to enhance the FFSGA methodology to overcome such shortcomings. For processes involving a large number of model inputs, other nonlinear techniques such as ANNs can be used to obtain an empirical model for the process or system under study.

Inductive models that result in a functional approximation of the response function tend to provide the added benefit of model parsimony. However, it should be realized that not all inductive models (including the ones developed by using FFSGA) are parsimonious in that they 1) improve function interpretability, 2) contain less parameters and/or variables, and 3) provide better generalization and interpolation capabilities. FFSGA allows the user the flexibility to control the complexity of the functional structure and parameters used. Depending on the choice of the internal functions of the model inputs, the resulting expressions from the FFSGA model vary in their parameter and functional complexity. Model complexity comes with improved accuracy, but it renders the model to be less parsimonious and functionally interpretable.

CHAPTER 5
MACRO-LEVEL WATER QUALITY SIMULATION MODELS

5.1 Introduction

An optimal management model for a watershed consists of two distinct components, 1) a water quality simulation model, and 2) an optimization model linked to the simulation model. Chapter 2 described the different types of water quality simulation models as well as optimization models that can be used in such a formulation. In theory, three different levels or types of macro-level models are possible in such a formulation namely 1) implicit inductive models, 2) explicit inductive models, and 3) simplified deductive models. This research will investigate the utility of explicit inductive and simplified deductive models in the context of an optimal watershed management framework. Macro-level models are simpler models that will be investigated for use as substitutes for complex deductive models and are discussed in detail in the following sections.

5.2 Macro-level Models in an Optimal Management Framework

Each water quality model has its own unique purpose and simulation characteristics and the preferred choice will depend on factors such as complexity of process being modeled, input data requirements, modeling objectives, and model applicability. In a complex watershed, the modeling objectives may require the use of a combination of models. In other cases, a very simplified representation of the processes or system under study might be sufficient to support the decision-making needs. For a complex watershed, it is often required to construct a series of deductive models to simulate multiple processes occurring in the watershed. For instance, both a watershed-scale loading as well as a receiving water model is needed for a watershed of sufficient complexity in which both point and non-point sources of pollution are being modeled. Moreover, multiple receiving water models of increasing complexity may be needed to model the transport of pollutants from the source to the receiving waters. Figure 5-1 shows one example of a series of models needed for a complex watershed.

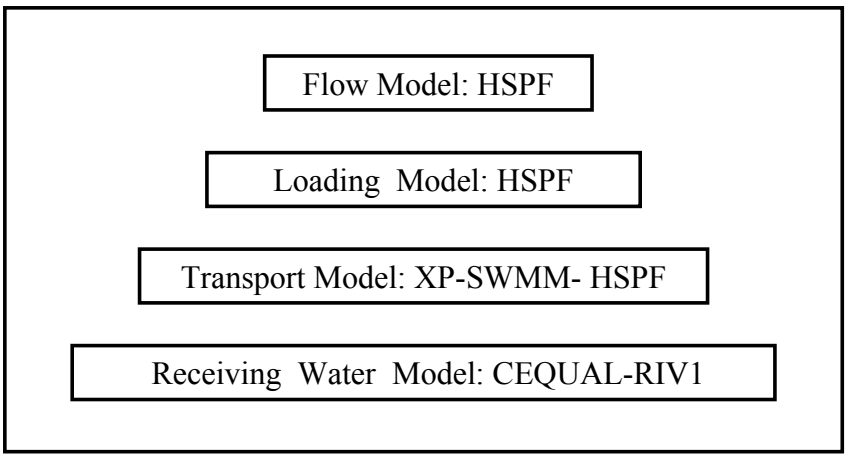


Figure 5-1. Simulation Models for a Complex Watershed

While such a series of deductive models are anticipated to better reflect the true dynamics of the process or processes being modeled, these can at times be cumbersome and complex. Such models require extensive knowledge of the process being modeled, require significant efforts in calibration and verification, and can be computationally very expensive. In particular, such models may not be ideally suited for application in a planning and water quality management framework in which multiple strategies would be evaluated in a short time. For instance, it may require more than 24 hours completing one simulation run of a series of models given in Figure 5-1. Linking such a series of models in an optimization framework can be very cumbersome and complex and will not allow for an efficient way to evaluate multiple management scenarios.

In an optimal management formulation for water quality management, quick and simple simulation models will be more favorable to evaluate multiple scenarios in a relatively short period of time. Such models can be very effective to support decision making on a planning level to formulate optimal strategies for water quality management in an urban watershed. Once an optimal strategy or strategies are selected to be suitable for a particular application, they can always be validated by a full blown deductive or process-based model of the watershed. To facilitate such a process, the concept of a *macro-level simulation model* is introduced here. Such a model is a simplified approach to modeling a response function of interest and is a macro-translation of the complex model or suite of models. Macro-level models can be effectively incorporated into a nonlinear

optimization framework for water quality management as shown in Figure 5-2. As stated previously, once an optimal strategy or set of strategies are selected for a particular application, they can be verified by using the more detailed and complex process-based model developed for the watershed. Three different levels or types of macro-level models can be used in such a formulation as given in Figure 5-3. These include 1) an implicit inductive model, 2) an explicit inductive model, and 3) a simplified deductive model. The choice of a particular model type depends on the particular application, available data, and the complexity of process or processes being modeled.

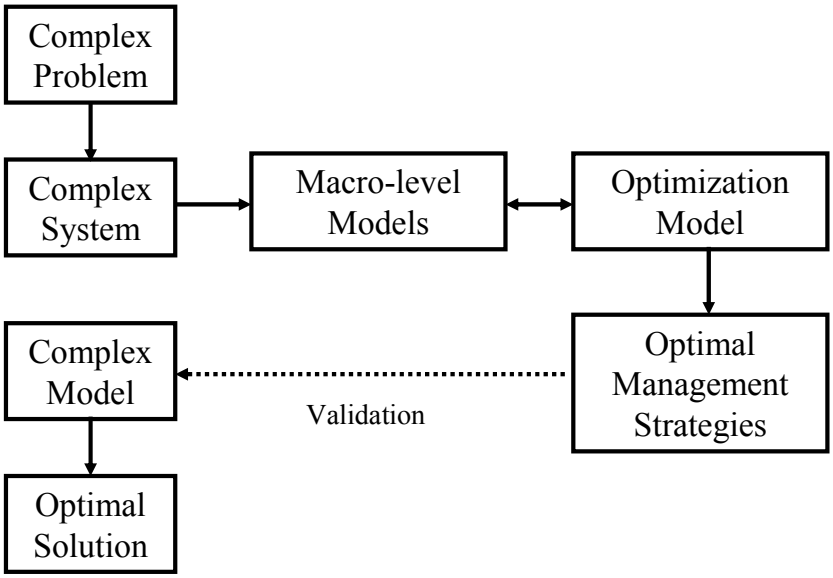


Figure 5-2. Water Quality Management using Macro-level Simulation models

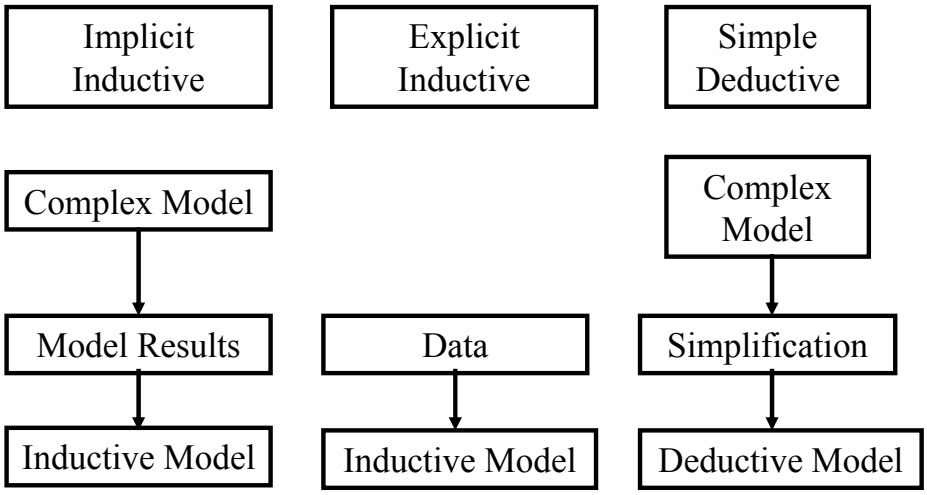


Figure 5-3. Types of Macro-Level Simulation Models

5.3 Inductive Simulation Models

Inductive or data-driven models are becoming more and more popular due to their ease of use and simplicity as substitutes for more process-based models in a number of applications. For instance, inductive models may be preferred where 1) computational expense is a critical issue, 2) the process-based deductive models are over parameterized and cannot be adequately calibrated, and 3) budgetary constraints do not allow for a complex deductive model (Tufail and Ormsbee, 2006). These factors led to the motivation of evaluating the utility of inductive models as macro-level transformation of the more complex deductive models and their subsequent use in an optimal management formulation. The following sections will describe the development of inductive simulation models for watershed management.

5.3.1 Implicit Inductive Models

An implicit inductive model is constructed by utilizing output data from a calibrated deductive model of the process or system being modeled. This approach can be useful in situations where 1) a fully calibrated deductive model is available but it is very complex for integrated into an optimization framework and thereby computationally expense, and

2) there is lack of raw data needed to develop an explicit inductive model. Implicit inductive models can result in significant computational savings and may be more favorable if quick decisions are needed over a short period of time.

The techniques used to construct such inductive models can vary from simple regression methods to more complex and non-linear evolutionary methods such as Artificial Neural Networks (ANNs), genetic programming (GP), and genetic functions (GFs). Muleta (2003) developed an ANN model to mimic SWAT (U.S. Department of Agriculture Soil and Water Assessment Tool) outputs and used the resulting inductive model in an optimal management model for controlling non-point source pollution. The real-world watershed used in this research is the Beargrass Creek watershed in Louisville, Kentucky. The fact that deductive models for the Beargrass Creek watershed are still under development did not allow for testing the utility of the implicit inductive approach in this research.

5.3.2 Explicit Inductive Models

An explicit inductive model can be constructed when sufficient data are available to permit the development of an inductive relationship between the independent and dependent variables. The development of explicit inductive models requires sufficient raw data over a range of time to fully capture the behavior of the response function being modeled. The use of explicit inductive models in an optimization framework can be a favorable choice due to their ease of use and simplicity as substitutes for more process-based deductive models. While such an approach can result in significant computational savings resulting in an efficient and effective optimal management framework, it is important to make sure that the resulting model is capable of accurately representing the response function. This can be verified by evaluating the assumed cause and effect relationship between input and output variables through the process of model validation. As in the case of implicit inductive models described above, the techniques used to construct explicit inductive models can vary from simple regression methods to more complex and non-linear evolutionary methods such as ANN, GP, and GFs.

Example applications of the explicit inductive model approach to watershed modeling are given as follows. These include the following three types of explicit inductive models:

1. Explicit inductive models for pathogens (fecal coliform).
2. Explicit inductive models for nutrients (total phosphorus and total nitrogen).
3. Explicit inductive models for dissolved oxygen (DO).

The nutrient and DO models were developed by utilizing data collected for the Beargrass Creek watershed in Louisville, Kentucky. For pathogen modeling, sufficient data was not available for the Beargrass Creek watershed at the time of this study, and thus data collected at the intake structure of a Water Treatment plant (Fayette County, Kentucky) on Kentucky River was used to demonstrate the utility of the explicit inductive modeling approach for pathogens. These three types of explicit inductive models are described as follow:

5.3.2.1 Explicit Inductive Models for Pathogens

The U.S. Environmental Protection Agency (USEPA) lists bacteria as primary water quality concern. Impairment of surface waters by fecal coliform bacteria is a water quality issue of national scope and importance (Moyer and Hyer, 2003). The presence of fecal coliform bacteria in surface water indicates fecal contamination and possibly the presence of other organisms that may be cause disease (Christensen, et al. 2000). Fecal coliform is a bacterium which can be found within the intestinal tract of all warm blooded animals. Fecal coliform can therefore be found in the fecal wastes of warm blooded animals. Fecal coliform in itself is not a pathogenic organism. However, fecal coliform indicates the presence of fecal wastes and the potential for the existence of other pathogenic bacteria. The higher concentrations of fecal coliform indicate the elevated likelihood of increased pathogenic organisms. Fecal coliform bacteria concentrations that are elevated above the state water quality standard indicate an increased risk to humans through swimming and other contact recreational activities.

Fecal coliform modeling continues to be a challenge due to the numerous sources of bacteria and the corresponding magnitudes of contributions from each source add to such challenges. In such challenging scenarios, the use of site specific inductive models based on water quality sampling data appears to be a promising choice. Explicit inductive models are developed in this study. The input to these models will include measured stream flows and turbidity. Turbidity is the measure of the cloudiness of a sample of water. Suspended matter, such as clay, silt, fine organic and inorganic matter, soluble organic compounds, and microscopic organisms, increases the turbidity of the water. Turbidity is measured by recording the amount of light scattered when a light beam passes through a sample of water. The instrument used to measure turbidity is called a nephelometer, and it records turbidity in units of nephelometric turbidity units (NTUs). Values of less than 10 NTU are desirable. Often, turbidity levels are positively correlated with water borne bacteria levels; as turbidity increases, bacterial levels increase. This phenomenon is typically due to the fact that surface runoff carries both suspended solids (silt, clay, and organic matter) as well as bacteria, so when it rains both the turbidity and the bacteria levels rise.

Three different inductive modeling techniques were used to develop explicit inductive models for pathogens. These include multiple linear regression, artificial neural networks (ANNs), and a fixed functional set genetic algorithm (FFSGA) approach to functional approximation. All ANN-based explicit inductive models were developed using a computer program called NEUROSORT (version 3.0) developed at the University of Kentucky (Lingreddy et al. 2003).

5.3.2.1.1 Study Area

The data used in developing inductive models for estimating fecal coliform concentration was extracted from a research report published by the Kentucky Water Resources Research Institute at the University of Kentucky (Brion et al. 2002). This data was collected at the raw water intake structure on Kentucky River for a water treatment plant in Lexington, Kentucky. The samples were collected at the intake site on the Kentucky

River between Lock 9 and Lock 10 as shown in Figure 5-4. The data collected included instantaneous stream flow, turbidity, water temperature, daily rainfall, and fecal coliform concentration. Due to the spatial variability of daily rainfall data, it was not used as an input to the inductive models. Initial screening of the raw data suggested a relationship between daily stream flows, turbidity, and fecal coliform concentration. Consequently, daily stream flow and turbidity were used as inputs to the inductive model, and fecal coliform is the target output to be predicted by the inductive models.

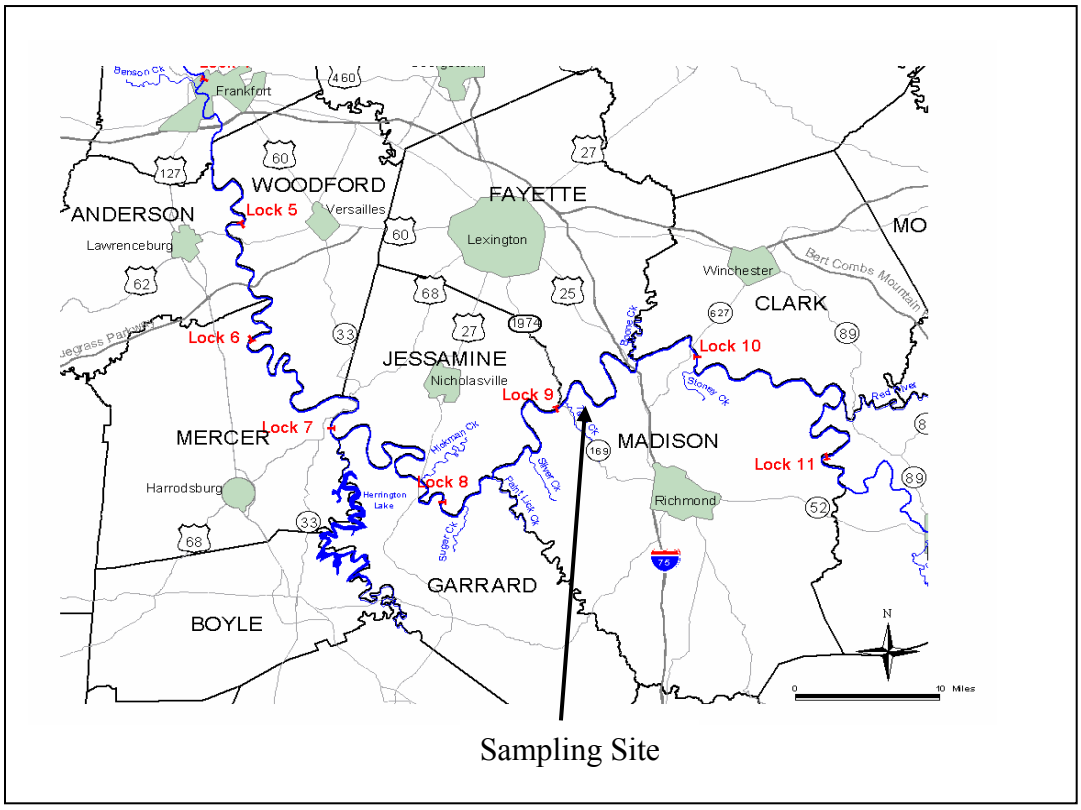


Figure 5-4. Sampling Site Location for data used in Inductive Pathogen Models

5.3.2.1.2 Data Statistics

The data used for analysis spans over a five year sampling period (1997 to 2001) and Table 5-1 gives a summary of the statistics of the data set used in this application. Per Kentucky Water Quality Standards, the monthly geometric mean of fecal coliform

bacteria in the recreational season (May 1 through October 31) is not to exceed 200 colonies per 100 ml or 20 percent or more of all samples taken in one month period are not to exceed 400 colonies per 100 ml (Kentucky Administrative Regulations Title 401, Chapter 5, Water Quality).

Table 5-1. May through October Statistics of the Data Set

Year	Average Q	Min Q	Max Q	Total Rain	Average FC	Maximum FC
	(cfs)	(cfs)	(cfs)	(inches)	(col/100 ml)	(col/100 ml)
1997	3910	140	41500	27.28	305	10000
1998	4005	158	23700	25.84	376	7700
1999	656	22	7360	11.79	16	296
2000	1802	160	13800	10.34	31	400
2001	2071	224	22500	24.82	120	3800

5.3.2.1.3 Development of Inductive Models

Two different types of models will be developed for pathogens. These include 1) a prediction model in which the model output will be the fecal concentration, and 2) a classification model in which the output will be the class of fecal concentration as defined below in Table 5-2.

Table 5-2. Classes of Fecal Coliform Concentration

Class or Group	Range of Fecal Concentration (col/100 ml)
1	0-200
2	200-400
3	400 and above

Predicting the class (i.e. the range of the fecal concentration) rather than the actual concentration can be beneficial when the actual concentration of fecal coliform is not required. For instance, in cases where early warning systems or advisories are needed to prevent people from contact with contaminated water, models capable of predicting the range of fecal coliform as opposed to the actual fecal coliform concentration can assist in minimizing the associated human health risks. For instance, such advisories and

warnings are routinely needed at recreational beaches to inform the public of potential health risks associated with such water bodies.

5.3.2.1.3.1 Regression Models

Linear multiple regression inductive models were developed for predicting fecal coliform concentration based on the daily stream flow and turbidity measurements collected at the site. The form of the multiple linear regression models is given as follows:

$$FC = a_0 + a_1 Q + a_2 T \qquad (5\text{-}1)$$

where a_0 through a_n are regression coefficients, Q (daily stream flow) and T (turbidity) are the independent variables in the regression model, and FC (fecal coliform concentration) is the dependent variable to be predicted by the model.

<u>Results of the Regression Models</u>

Regression models to estimate fecal coliform concentration were developed using the 1997 through 2000 data set and validated by using the 2001 data set. Two different types of prediction models were developed including:

- Model A in which the actual values of flow, turbidity, and fecal concentration were used in model development and
- Model B in which the logarithmic values of flow, turbidity, and fecal concentration were used in model development.

The log transformation has a significant effect on the performance of the models as demonstrated in the results to follow. The resulting regression equations for the two types of prediction models are given in Equation 5-2 and 5-3.

$$FC = -16 + 0.023Q + 3.36T \qquad (5\text{-}2)$$

$$\log_{10} FC = -0.055 \log_{10} Q + 1.249 \log_{10} T \qquad (5\text{-}3)$$

Figures 5-5 through 5-8 give the time series of fecal coliform monthly geometric mean for the two types of regression models (Model A and B) in training and validation. Table 5-3 gives a summary of results for the regression-based prediction models including average absolute error, maximum absolute error, mean square error (MSE), and coefficient of determination (R^2) for predicting the concentration of fecal coliform concentration for both model training and validation. Results are given for both model structure A and B. Table 5-4 gives a comparison of the performance of regression-based prediction and classification models in successfully predicting the class of fecal coliform concentration as identified in Table 5-2.

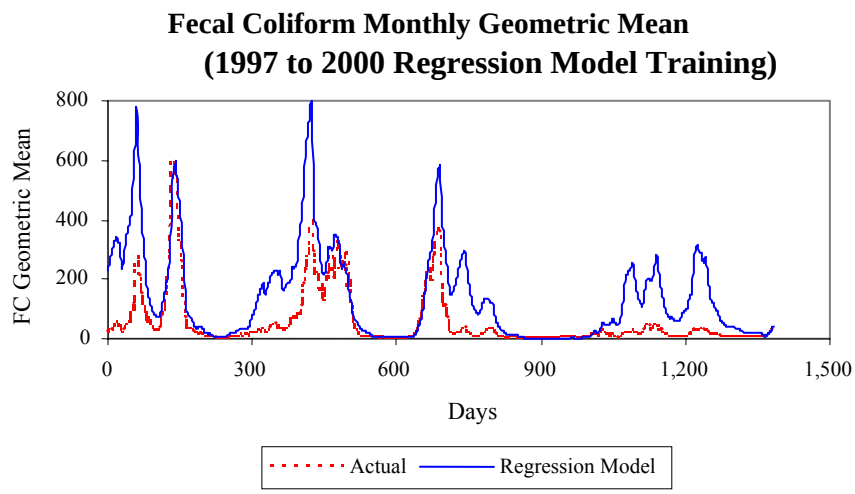


Figure 5-5. Time Series of Fecal Coliform Monthly Geometric Mean (Model "A" Training)

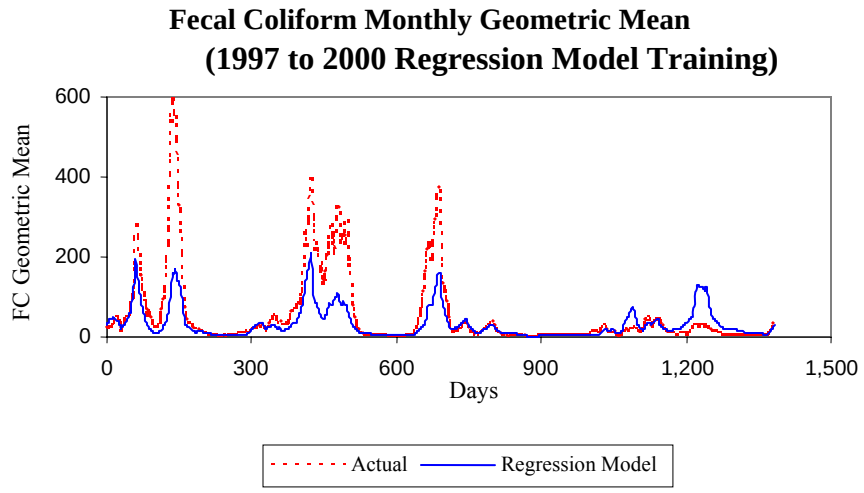


Figure 5-6. Time Series of Fecal Coliform Monthly Geometric Mean (Model "B" Training)

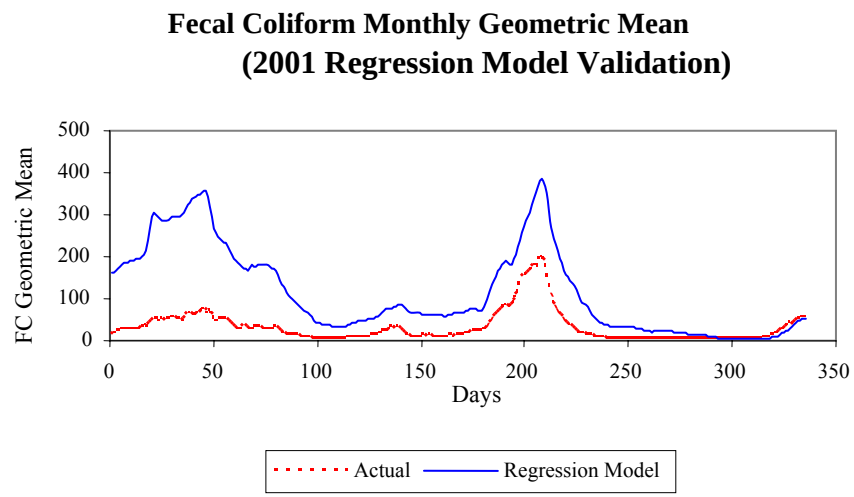


Figure 5-7. Time Series of Fecal Coliform Monthly Geometric Mean (Model "A" Validation)

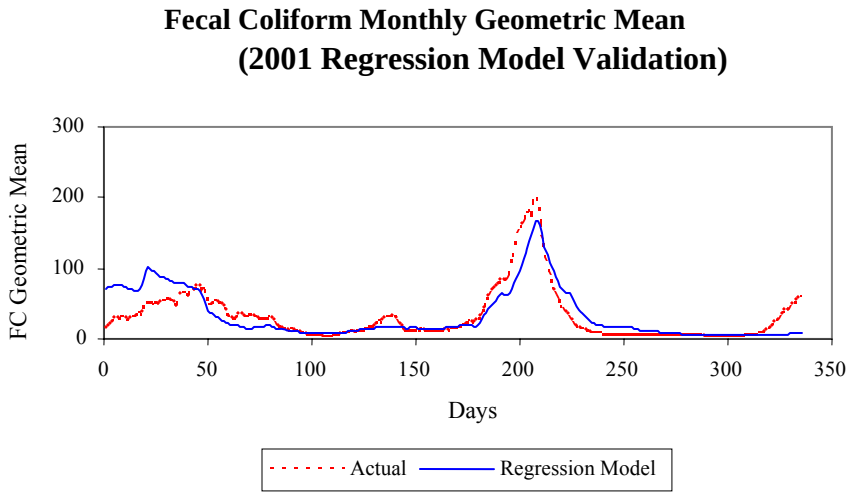


Figure 5-8. Time Series of Fecal Coliform Monthly Geometric Mean (Model "B" Validation)

Table 5-3. Results Summary of Regression-Based Prediction Models

Data Set Description Model Performance	**1997-2000 Training(1)**	**2001 Validation(1)**	**1997-2000 Training(2)**	**2001 Validation(2)**
# of Data	1,382	336	1,382	336
Average Absolute Error (Monthly Geometric Mean)	89	85	30	14
Maximum Absolute Error (Monthly Geometric Mean)	560	282	440	61
Mean Square Error (MSE) (Monthly Geometric Mean)	18,338	13,143	4,212	431
Coefficient of Determination (R^2) (Monthly Geometric Mean)	0.58	0.62	0.66	0.69

(1): Actual data (flow, turbidity, and fecal concentration) used in the development of the model.
(2): Logarithmic transformed data (log flow, log turbidity, log fecal concentration) used in the development of the model.

Table 5-4. Comparison of Regression-Based Prediction and Classification Models

Data Set Description Model Performance	**1997-2000 Training(1)**	**2001 Validation(1)**
# of Data	1,382	336
% Success (Prediction Model)	79%	77%
% Success (Classification Model)	84%	86%

(1): Actual data (flow, turbidity, and fecal concentration) used in the development of the model.

It is interesting to note that the model results improve significantly when the logarithmic transformed data is used in the training and subsequent validation of the model. Log transformation is a technique often used in regression analysis as it improves the performance and prediction ability of the resulting models. This is particularly true for cases where there is significant variability (volatility) in the raw data, and the use of log-transformed regression is recommended because it provides the most stable estimation. For instance, the regression models developed by Christensen, et al. (2000; 2002) also result in expressions that predict the log transformed values of fecal concentration.

5.3.2.1.3.2 ANN Models

The popular multi layer feed-forward back propagation neural networks were used in developing inductive models for fecal coliform bacteria modeling. The model structure included one input layer, one hidden layer, and a corresponding output layer. The input layer consists of two input nodes representing daily stream flow (Q) and turbidity (T) whereas the output layer consist of one node representing the target fecal coliform bacteria concentration (FC). The number of hidden nodes (H) in the hidden layer was varied in the model development, starting with two nodes and going up to a maximum of six nodes. A general schematic of the ANN structure used in developing the fecal coliform inductive models is given below in Figure 5-9.

The ANN network architecture was varied by trying different number of hidden nodes in the hidden layer and varying the learning rate and momentum rate parameters. The learning rate is a factor that determines the amount by which the connection weight is changes according to error gradient information. The momentum parameter governs the weight change in the current iteration of the algorithm due to change in the previous iteration. These factors are obtained by trial and error method (Zurada, 1992). In the majority of evaluations, the most optimal results were obtained by using two hidden nodes in the hidden layer. The ANN structure used for fecal modeling used a logistic sigmoid function of the form given as:

$$f(x) = \frac{1}{1+e^{-x}} \qquad (5\text{-}4)$$

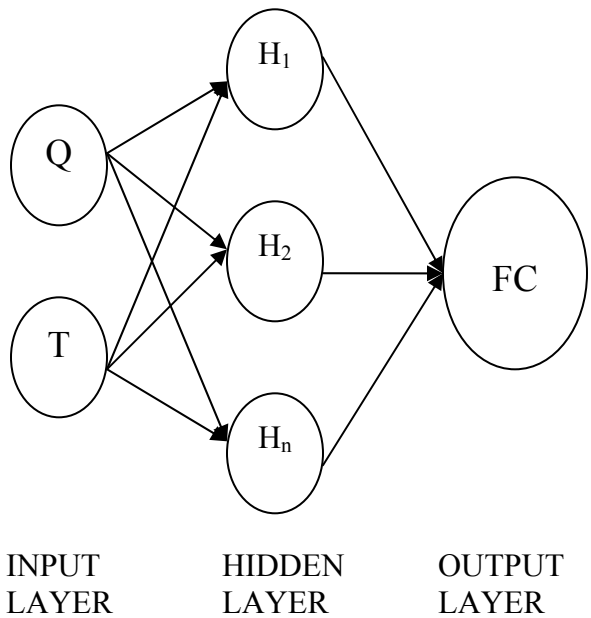


Figure 5-9. Neural Network Structure for Inductive Pathogen Models

Results of the ANN-based Inductive Models

ANN models to estimate fecal coliform concentration were developed using the 1997 through 2000 data set and validated by using the 2001 data set. As in the case of the regression models, two types of prediction models (Model A and Model B) were developed, one using the raw data (actual values of flow, turbidity, and fecal concentration), and the other using the log-transformed values of these variables. The log transformation improves the performance of the models as will be seen in the results to follow. This improvement is not as significant as was seen in the case of the regression models. Figures 5-10 through 5-13 give the time series of fecal coliform monthly geometric mean obtained in training and validation for model types A and B. Table 5-5 gives a summary of results for the ANN-based prediction model including average absolute error, maximum absolute error, mean square error (MSE), and coefficient of

determination (R^2) for predicting the concentration of fecal coliform concentration for both model training and validation. Results are given for both model structure A and B. Table 5-6 gives a comparison of the performance of ANN-based prediction and classification models in successfully predicting the class of fecal coliform concentration as identified in Table 5-2.

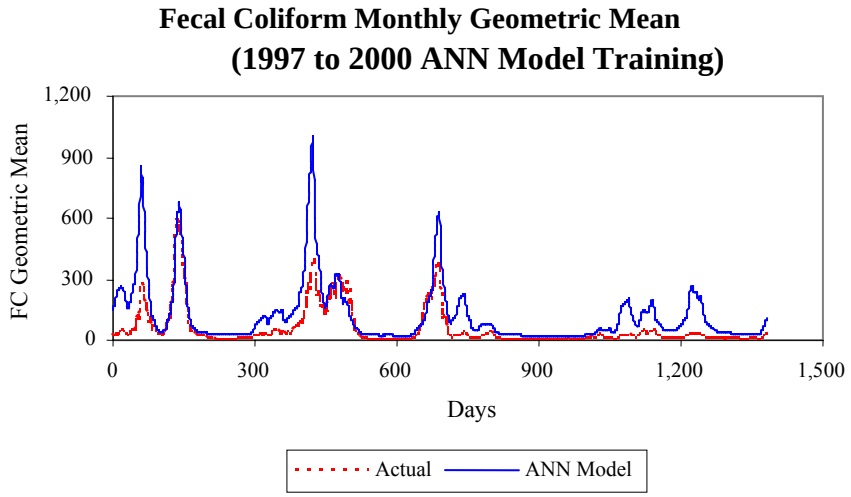


Figure 5-10. Time Series of Fecal Coliform Monthly Geometric Mean (Model "A" Training)

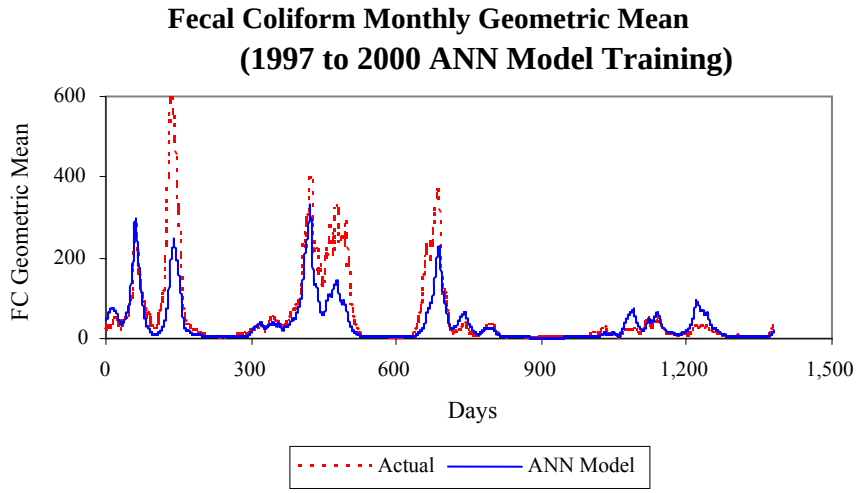


Figure 5-11. Time Series of Fecal Coliform Monthly Geometric Mean (Model "B" Training)

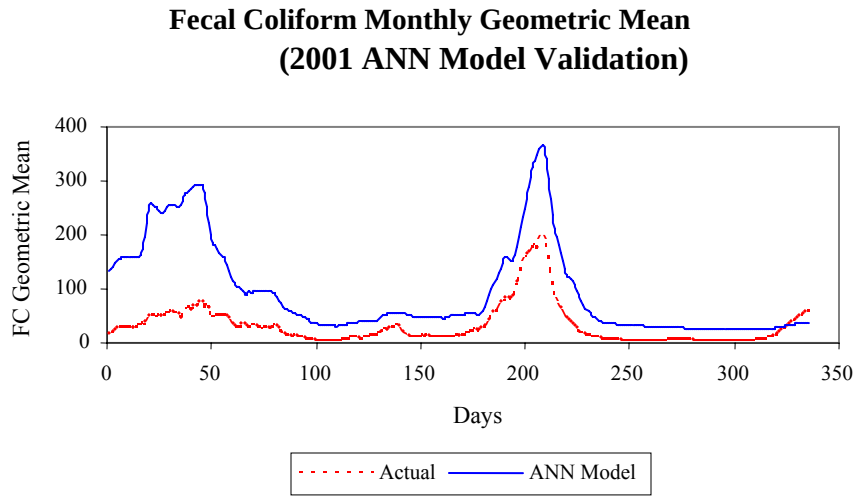


Figure 5-12. Time Series of Fecal Coliform Monthly Geometric Mean (Model "A" Validation)

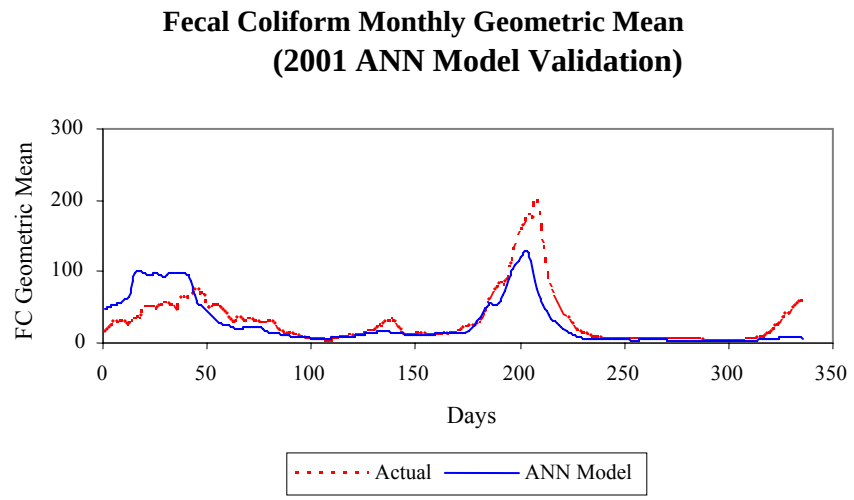


Figure 5-13. Time Series of Fecal Coliform Monthly Geometric Mean (Model "B" Validation)

Table 5-5. Results Summary of ANN-Based Prediction Models

Data Set Description **Model Performance**	**1997-2000** **Training(1)**	**2001** **Validation(1)**	**1997-2000** **Training(2)**	**2001** **Validation(2)**
# of Data	1,382	336	1,382	336
Average Absolute Error (Monthly Geometric Mean)	74	64	24	13
Maximum Absolute Error (Monthly Geometric Mean)	616	228	387	71
Mean Square Error (MSE) (Monthly Geometric Mean)	13,974	7,551	2,852	441
Coefficient of Determination (R^2) (Monthly Geometric Mean)	0.66	0.70	0.73	0.58

(1): Actual data (flow, turbidity, and fecal concentration) used in the development of the model.
(2): Logarithmic transformed data (log flow, log turbidity, log fecal concentration) used in the development of the model.

Table 5-6. Comparison of ANN-Based Prediction and Classification Models

Data Set Description **Model Performance**	**1997-2000** **Training(1)**	**2001** **Validation(1)**
# of Data	1,382	336
% Success (Prediction Model)	83%	80%
% Success (Classification Model)	85%	87%

(1): Actual data (flow, turbidity, and fecal concentration) used in the development of the model.

5.3.2.1.3.3 FFSGA Models

Fixed Functional Set Genetic Algorithm (FFSGA) approach of inductive modeling is particularly suited for cases in which a simple and easy to use functional form is sought to represent the response function being modeled. The FFSGA approach starts with a pre-defined functional form which is a combination of numeric coefficients, sub-functions of decision variables (model inputs), and mathematical operators. In the first step, the GA searches for the optimal sub-functions of the decision variables and mathematical operators to obtain the optimal functional components that will constitute the structure of the desired functional form. In the second step, the coefficients of the functional form are obtained by least squares optimization. In the present application, the objective function is the optimal functional form sought for the fecal coliform bacteria concentration in terms of the two model inputs (i.e. daily stream flow Q and turbidity T)

and the fitness function is based on the mean square error (MSE) of the performance of the objective function in predicting the target fecal concentration values. Five different fixed functional forms were formulated to represent the expression for fecal coliform concentration as given in Figure 5-14 (these represent the general form of the empirical expressions sought), each being some combination of elementary sub-functions of the two independent variables. These forms also consist of coefficients that act as weighting factors for the sub-functions of the independent variables. These coefficients will be obtained using least squares optimization after the GA search process identifies the optimal sub-functions to be used in the expression sought. Table 5-7 gives a list of a sample of 15 different sub-functions for each of the decision variables (model inputs) that are available for selection by the FFSGA model. The number of such elementary sub-functions can be expanded further by introducing more functions or combination of functions. A larger set of available functions will facilitate the GA search process by providing greater diversity and selection. Table 5-8 gives the corresponding mathematical operators that are available for selection by the FFSGA model.

Functional Form #1 = {C_1 operator_1 [function_1 (Q) operator_2 function_2 (T)]} operator_3
{C_2 operator_4 [function_3 (Q) operator_5 function_4 (T)]}

Functional Form #2 = {C_1 * [function_1 (Q) operator_1 function_2 (T)]} operator_2
{C_2 * [function_3 (Q) operator_4 function_4 (T)]}

Functional Form #3 = {C_1 * function_1 (Q) * function_2 (T)} operator_1
{C_2 * function_3 (Q) * function_4 (T)}

Functional Form #4 = {C_1 * function_1 (Q)} operator_1 {C_2 * function_2 (T)}

Functional Form #5 = {[C_1 * function_1 (Q)] operator_1 [C_2 * function_2 (T)]} operator_2
{C_3 * function_3 (Q) * function_4 (T)}

Figure 5-14. Pre-defined FFSGA Functional Forms for Inductive Pathogen Models

Table 5-7. List of functions for Flow (Q) and Turbidity (T)

Function #	Function f (Q) or Function f (T)
1	1
2	Q or T or Sqrt(Q) or Sqrt(T)
3	1/Q or 1/(T)
4	Exp (Q) or Exp (T)
5	Log_e (Q) or Log_e (T)
6	Log_{10} (Q) or Log_{10} (T)
7	Exp (1/Q) or Exp (1/T)
8	Log_e (1/Q) or Log_e (1/T)
9	Log_{10} (1/Q) or Log_{10} (1/T)
10	Q*Exp(Q) or T*Exp(T)
11	Q* Log_e (Q) or T*Log_e (T)
12	Q*Log_{10} (Q) or T*Log_{10} (T)
13	(1/Q)*Exp(Q) or (1/T)*Exp(T)
14	(1/Q)* Log_e (Q) or (1/T)*Log_e (T)
15	(1/Q)*Log_{10} (Q) or (1/T)*Log_{10} (T)

Table 5-8. List of Operators in the General Functional Forms

Operator #	Operator
1	+
2	-
3	*
4	/
5	^

The FFSGA model evaluates each of the five functional forms (Figure 5-14) individually. In each case, the model starts with a random selection of solution sets resulting in an initial population of solutions, each comprised of a set of functions (from Table 5-7) and operators (from Table 5-8). Each solution set thus represents an explicit equation for fecal coliform concentration. These solution sets are evaluated for the given data set (values of Q and T in this case) and the predicted values of fecal coliform concentration are compared against the target or actual fecal coliform concentration values to determine the mean square error (MSE). The MSE is a measure of how good the given solution set is in representing the data set evaluated and translates into the corresponding fitness function. The FFSGA model continues to evolve new set of solution vectors as the search marches from one generation to the other. At the termination of specified generations, the functional form that has the highest fitness value is the optimal structure

of the explicit expression sought in the search process. Finally, the coefficients of the functional form are obtained by applying least squares optimization to the optimal form obtained from the GA process.

Results of the FFSGA-based Inductive Models

FFSGA models to estimate fecal coliform concentration were developed using the 1997 through 2000 data set and validated by using the 2001 data set. As in the case of regression and ANN-based models, two types of models (A and B) were developed, one uses the raw data and the other uses the log-transformed values of the variables. The log transformation improves the performance of the models as will be seen in the results to follow. FFSGA identified two optimal expressions, one for the actual data (model type A) and one for the log transformed data (model type B) and these are given as Equations 5-5 and 5-6.

$$FC = \frac{21.1935 * [SQRT(Q)]}{35.129 * \left[SQRT\ (\frac{1}{T}) \right]} \tag{5-5}$$

$$Log_{10}FC = \frac{-49.2581 * \lfloor SQRT\ (Log_{10}\ Q) \rfloor}{-83.5161 * \left[\frac{1}{Log_{10}\ T} \right]} \tag{5-6}$$

The performance of the FFSGA-based models is demonstrated in Figures 5-15 through 5-18 in which the time series of fecal coliform monthly geometric mean during training and validation are given. Table 5-9 gives a summary of results for the FFSGA-based prediction models including average absolute error, maximum absolute error, mean square error (MSE), and coefficient of determination (R^2) for predicting the concentration of fecal coliform concentration in both model training and validation. Results are given for both model structure A and B. Table 5-10 gives a comparison of the performance of

FFSGA-based prediction and classification models in successfully predicting the class of fecal coliform concentration as identified in Table 5-2.

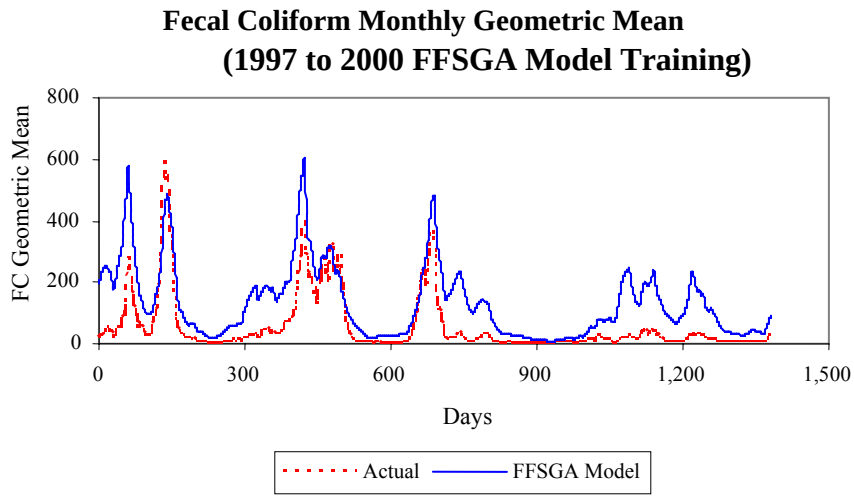


Figure 5-15. Time Series of Fecal Coliform Monthly Geometric Mean (Model "A" Training)

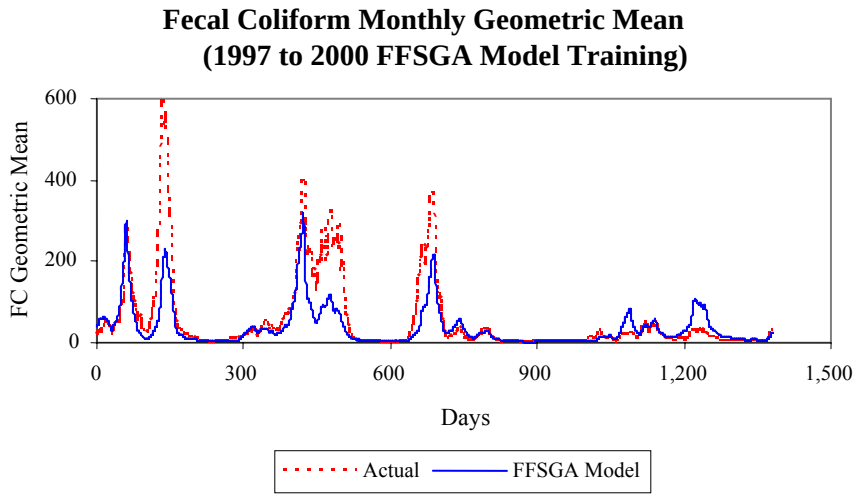


Figure 5-16. Time Series of Fecal Coliform Monthly Geometric Mean (Model "B" Training)

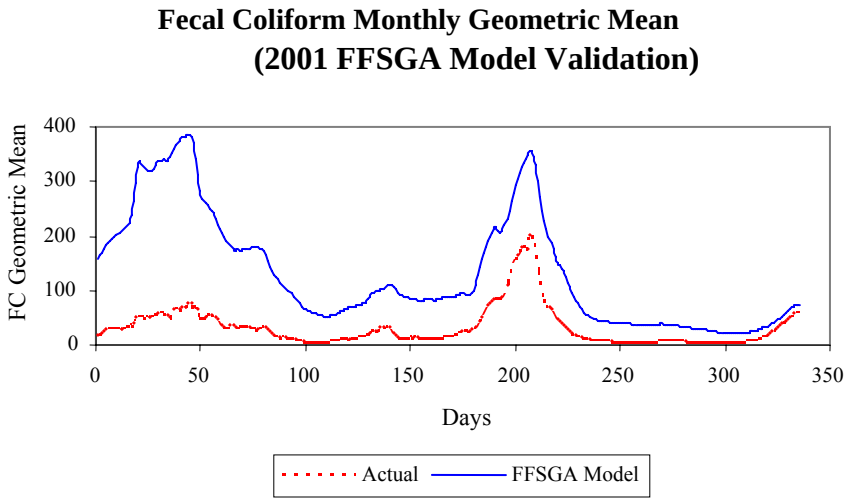


Figure 5-17. Time Series of Fecal Coliform Monthly Geometric Mean (Model "A" Validation)

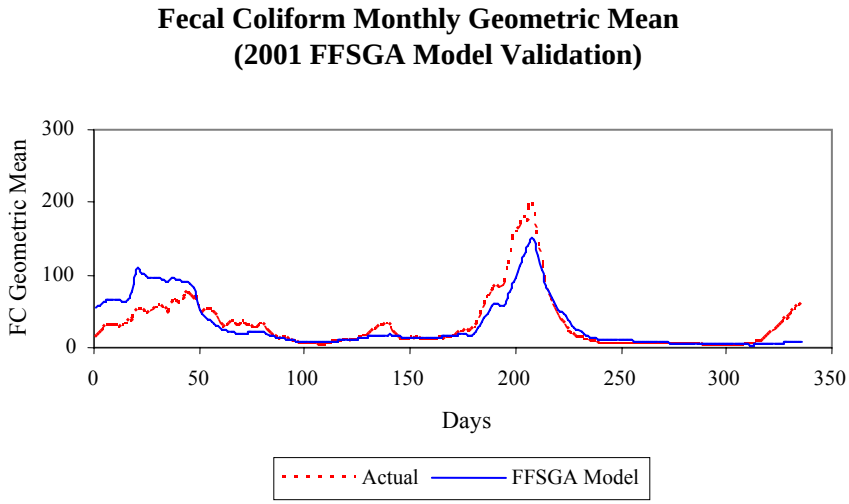


Figure 5-18. Time Series of Fecal Coliform Monthly Geometric Mean (Model "B" Validation)

Table 5-9. Results Summary of FFSGA-Based Prediction Models

Data Set Description Model Performance	1997-2000 Training(1)	2001 Validation(1)	1997-2000 Training(2)	2001 Validation(2)
# of Data	1,382	336	1,382	336
Average Absolute Error (Monthly Geometric Mean)	83	100	26	13
Maximum Absolute Error (Monthly Geometric Mean)	387	318	393	62
Mean Square Error (MSE) (Monthly Geometric Mean)	11,543	16,240	3,203	409
Coefficient of Determination (R^2) (Monthly Geometric Mean)	0.64	0.58	0.70	0.70

(1): Actual data (flow, turbidity, and fecal concentration) used in the development of the model.
(2): Logarithmic transformed data (log flow, log turbidity, log fecal concentration) used in the development of the model.

Table 5-10. Comparison of FFSGA-Based Prediction and Classification Models

Data Set Description Model Performance	1997-2000 Training(1)	2001 Validation(1)
# of Data	1,382	336
% Success (Prediction Model)	82%	84%
% Success (Classification Model)	84%	87%

(1): Actual data (flow, turbidity, and fecal concentration) used in the development of the model.

5.3.2.1.4 Summary of Results for Pathogen Models

Fecal coliform modeling is challenging owing to the significant variability in its source and magnitude. This is encountered in both inductive and deductive modeling approaches. The use of inductive techniques to develop pathogen models given an adequate set of sampled water quality data is becoming increasingly popular. Some of the recent work in this area includes the use of regression techniques in developing inductive models to estimate fecal concentration in surface water bodies (Christensen, et al. 2000). There were some significant findings in the development of inductive models for fecal coliform in the current work as described above. The model results show that log transformation of the input data removes the significant variability in the magnitude of fecal concentration. As a result, the three techniques are not significantly different in performance as seen in the results. It is worth mentioning that while regression results in a simple and linear model, ANN and FFSGA are highly nonlinear techniques capable of

capturing significant variability in the data. A comparison of the coefficient of determination (R^2) computed for the three techniques in predicting the 30-day geometric mean of fecal coliform reveal that for model structure "A", the ANN-based model performed slightly better than the other two techniques. For model structure "B", the FFSGA-based model performed slightly better than the other two techniques. Figures 5-19 through 5-22 gives a combined graph of the model results obtained using the three techniques in model training and validation for the two model structures "A" and "B".

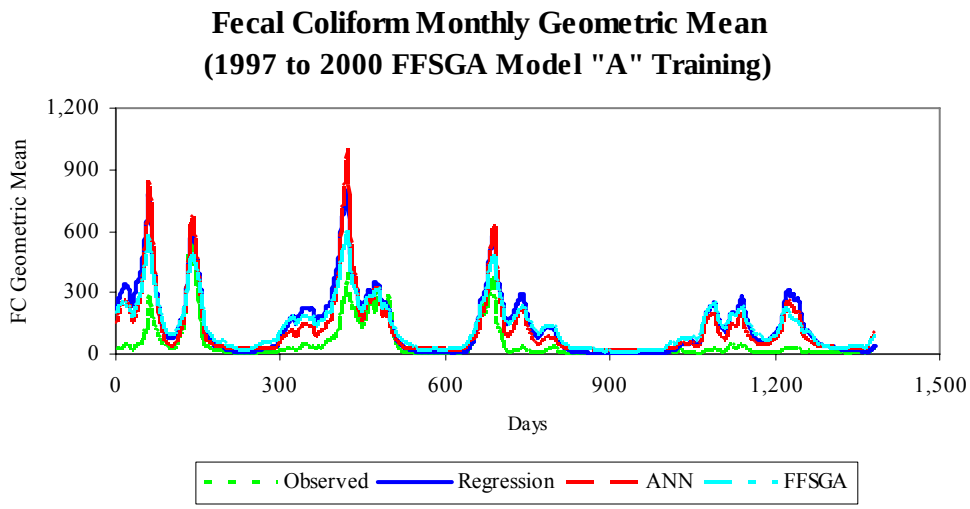


Figure 5-19. Comparison of Model Performance for Model Structure "A" Training

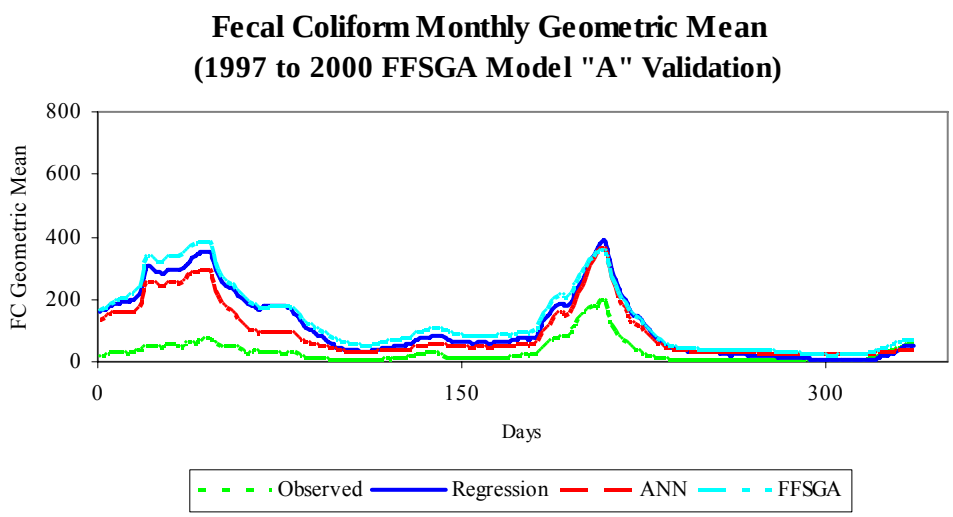


Figure 5-20. Comparison of Model Performance for Model Structure "A" Validation

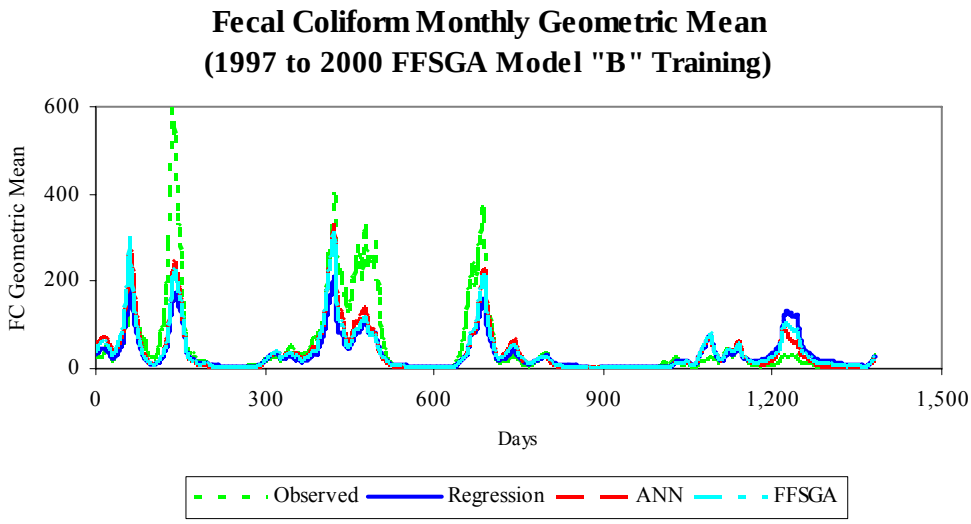


Figure 5-21. Comparison of Model Performance for Model Structure "B" Training

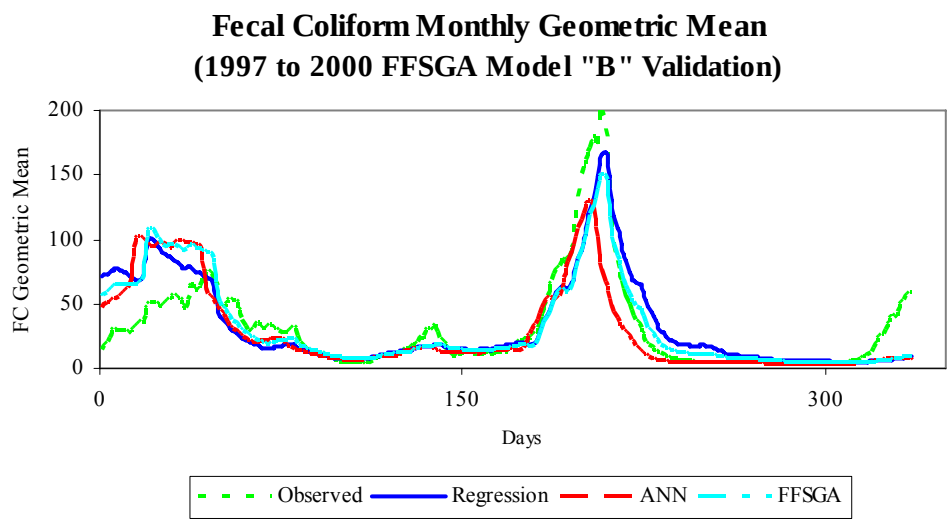


Figure 5-22. Comparison of Model Performance for Model Structure "B" Validation

Another significant finding of this work is the utility of predicting the class of fecal concentration in a given numeric range as opposed to the prediction of the actual numeric concentration. Given the significant variability in the magnitude and source of fecal concentration, it might be more beneficial to predict the class of fecal concentration as opposed to actual concentration. Such a class prediction can be of utility in monitoring

water quality in surface water bodies designated for contact recreation and issuing advisories and early warnings to minimize health hazards associated with contaminated waters. In the current work, the class of fecal concentration (as classified in Table 5-2) can be obtained either using the prediction model (in which the actual fecal concentration is predicted) or using the classification model (in which the class of fecal concentration is predicted). When the performance of the three inductive models is compared in predicting the class of fecal coliform, the more complex methods (ANN and FFSGA) performed slightly better than the simple regression method. This is demonstrated in a comparison of the performance of the three models in Table 5-11.

Table 5-11. Comparison of Model Performance in Fecal Classification

Data Set Description / Model Performance	% Success in Fecal Classification 1997-2000 Training(1)	% Success in Fecal Classification 2001 Validation(1)	% Success in Fecal Classification 1997-2000 Training(2)	% Success in Fecal Classification 2001 Validation(2)
Regression Model	79%	77%	84%	86%
ANN Model	83%	80%	85%	87%
FFSGA Model	82%	84%	84%	87%

(1): Results are based on the fecal coliform "prediction" models.
(2): Results are based on the fecal coliform "classification" models.

The results of the three inductive models (regression, ANNs, and FFSGA) for estimating fecal coliform concentration are very encouraging given the difficulty of fecal modeling. It can be synthesized that regression models are simple but can be very useful and should always be explored as a starting point before using more complex models. Data sets representing different physical processes vary from one to another. While non-linearity and complexity in some data sets may require more complex techniques such as those based on AI, simple regression methods continue to serve as a useful tool in most applications. The performance of the new GA-based method (FFSGA) is encouraging when compared to ANN. The greatest advantage of FFSGA approach (in comparison to ANN) is that it can generate simple, compact, and easy to use expressions that can be effectively used in estimating fecal coliform concentration.

5.3.2.2 Explicit Inductive Models for Nutrients

Explicit inductive models were developed to predict nutrients loads in each of the three forks of the Beargrass Creek watershed. These are described as follows.

5.3.2.2.1 Study Area

The Beargrass Creek watershed has multiple stream segments that are listed on the State's 303(d) list for low dissolved oxygen and/or nutrient enrichment as shown in Figure 5-23 below. Per Kentucky Water Quality Standards, the dissolved oxygen criterion for aquatic life is 5.0 mg/L (daily average) and 4.0 mg/L (instantaneous minimum) (Kentucky Administrative Regulations Title 401, Chapter 5, Water Quality). These include all of the South Fork and the lower reaches of the Middle Fork. A comprehensive water quality sampling program is in place for this watershed that includes both continuous water quality monitoring and discrete sampling for key parameters. The continuous sampling include DO meters that samples data every 15 minutes. The discrete sampling data include parameters such as total nitrogen and total phosphorus, which is hypothesized to be the main causes of low DO in the stream segments.

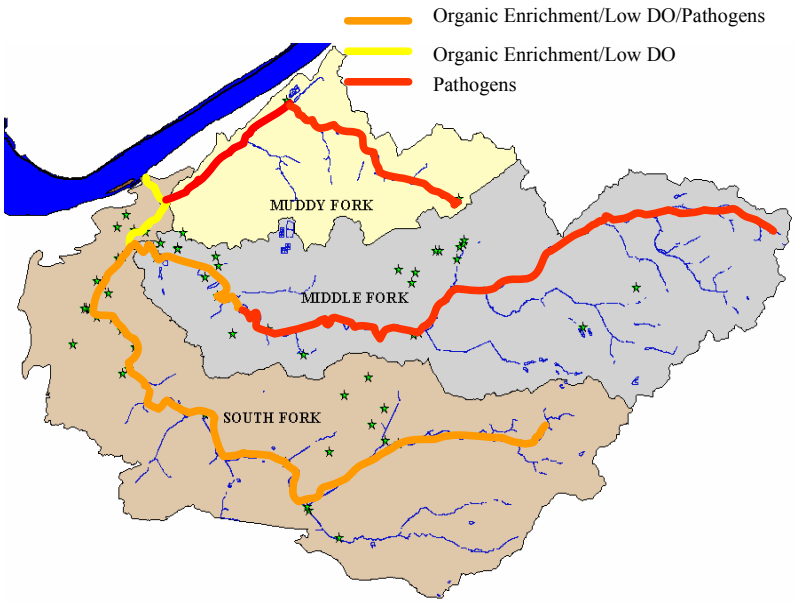


Figure 5-23. Beargrass Creek watershed: Causes of Impairment

5.3.2.2.2 Development of Inductive Models

Three different inductive modeling techniques namely regression, ANNs, and FFSGA were used to construct inductive models of watershed response for nutrients. These models will be used to determine the total nitrogen and total phosphorus loads generated by each of the three forks of the watershed. Nutrients are considered to be the main cause of the low dissolved oxygen (DO) in the impaired streams of the Beargrass Creek watershed (Figure 5-23). The nutrient models were developed using discrete water quality data collected at discrete sampling locations on the three forks of the watershed. Total nitrogen and total phosphorus concentration data (in MG/L) collected at these locations was used in conjunction with stream flows (in CFS) recorded at the same locations to compute the corresponding nutrient loads (flow multiplied by the concentration measured in total pounds per day). The nutrient loads thus computed were used as outputs in the inductive model with stream flows and conductivity used as inputs to the model.

Separate models were developed for the three monitoring locations (one in each of the three sub-watersheds of Beargrass Creek watershed) to characterize the nutrient loads from all the three sub-watersheds. These monitoring stations are shown in Figure 5-24 and described as follows:

1. Sampling site EMUMU001 on the Muddy Fork of Beargrass Creek
2. Sampling site EMIMI010 on the Middle Fork of Beargrass Creek
3. Sampling site ESFSF006 on the South Fork of Beargrass Creek

Note that site ESFSF006 is located downstream of the confluence of Middle and South Forks of the Beargrass Creek. Tables 5-12 through 5-14 give the raw data for these three sites.

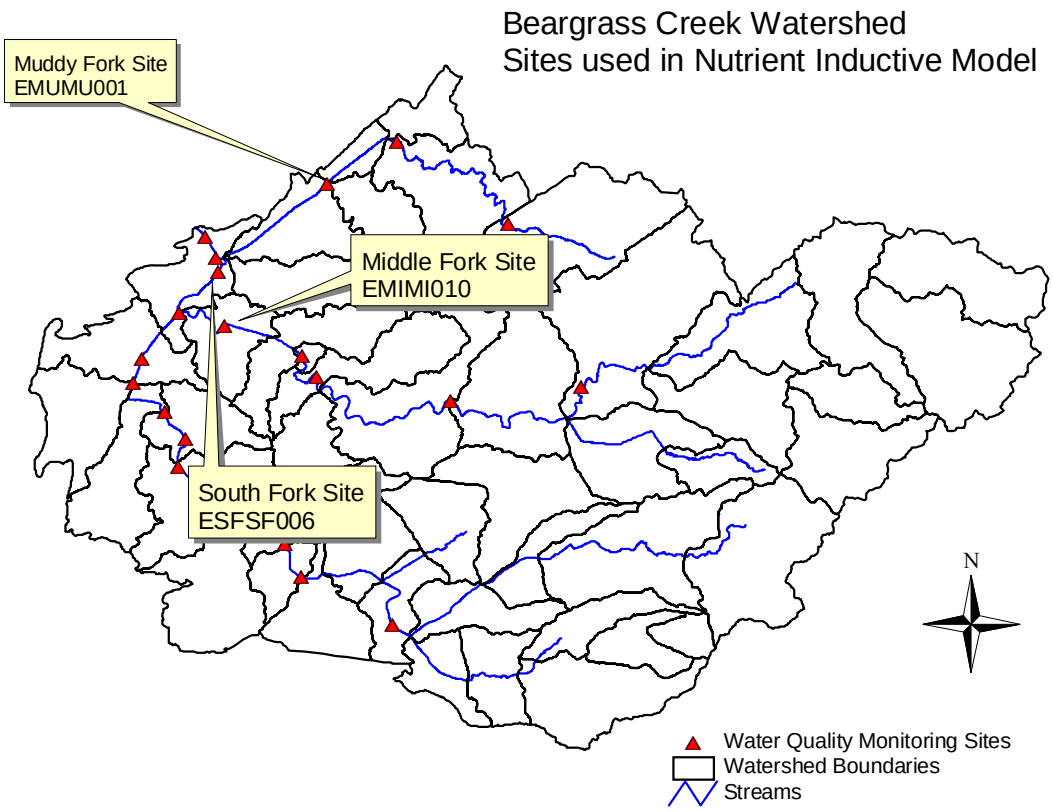


Figure 5-24. Discrete Sampling Sites used in Inductive Nutrient Models

Table 5-12. Discrete Sampling Data for Site ESFSF006

Data #	Date	Time	TN (mg/L)	TP (mg/L)	Conductivity (aes/cm)	Flow (cfs)	TN Load (lbs/d)	TP Load (lbs/d)
1	03/03/04	9:25:00 AM	2.23	0.05	647	49	591	14
2	03/03/04	1:45:00 PM	2.11	0.04	656	74	837	15
3	03/03/04	1:45:00 PM	0.52	0.04	656	74	205	15
4	03/03/04	2:25:00 PM	2.06	0.07	660	82	914	32
5	03/03/04	3:25:00 PM	4.82	0.60	660	88	2291	283
6	03/04/04	2:05:00 PM	2.00	0.22	683	451	4846	539
7	03/04/04	2:06:00 PM	1.87	0.22	683	451	4531	537
8	03/04/04	6:05:00 PM	2.73	0.21	692	294	4315	329
9	04/12/04	11:05:00 AM	0.52	0.03	705	14	39	2
10	04/12/04	11:05:00 AM	0.52	0.03	705	14	39	3
11	04/12/04	12:20:00 PM	1.37	0.27	698	33	242	47
12	04/12/04	2:05:00 PM	2.19	0.62	677	64	752	213
13	04/14/04	3:45:00 AM	2.33	0.45	369	409	5126	999
14	04/14/04	3:45:00 AM	2.21	0.43	369	409	4862	957
15	04/14/04	7:20:00 AM	2.11	0.26	399	285	3229	402
16	04/20/04	6:40:00 AM	1.95	0.14	715	31	327	24
17	04/20/04	10:00:00 AM	0.52	0.03	715	31	87	5
18	04/20/04	10:05:00 AM	0.52	0.03	715	31	87	5
19	04/21/04	11:35:00 AM	2.12	0.05	729	34	386	8
20	04/21/04	12:55:00 PM	2.16	0.20	636	142	1644	153
21	04/22/04	2:40:00 PM	2.16	0.39	443	102	1187	212
22	04/22/04	2:40:00 PM	2.35	0.30	443	102	1295	167
23	04/22/04	10:00:00 PM	1.86	0.22	510	78	787	92
24	04/23/04	1:15:00 AM	2.24	0.18	541	64	770	60
25	05/14/04	4:35:00 PM	0.52	0.03	686	20	55	3
26	05/14/04	4:37:00 PM	0.52	0.03	685	20	55	3
27	05/14/04	5:55:00 PM	2.11	0.15	677	73	831	60
28	05/14/04	7:35:00 PM	5.17	0.79	503	129	3605	553
29	05/15/04	7:55:00 PM	1.58	0.17	528	206	1752	188
30	05/15/04	7:56:00 PM	1.52	0.17	528	206	1685	185

Table 5-13. Discrete Sampling Data for Site EMUMU001

Data #	Date	Time	TN (mg/L)	TP (mg/L)	Conductivity (aes/cm)	Flow (cfs)	TN Load (lbs/d)	TP Load (lbs/d)
1	3/3/04	9:08 AM	2.24	0.03	662	61	735	11
2	3/3/04	12:40 PM	0.52	0.03	667	63	175	10
3	3/3/04	1:06 PM	2.14	0.03	667	64	737	10
4	3/3/04	1:26 PM	2.13	1.03	667	62	710	344
5	3/3/04	2:50 PM	2.50	0.03	668	70	941	11
6	3/4/04	1:46 PM	2.56	0.09	534	140	1928	64
7	3/4/04	1:47 PM	2.56	0.08	534	140	1928	61
8	3/4/04	5:55 PM	3.27	0.06	588	129	2270	42
9	4/12/04	10:45 AM	0.52	0.01	666	21	58	1
10	4/12/04	10:45 AM	0.52	0.03	666	21	58	3
11	4/12/04	12:00 PM	1.85	0.10	658	27	269	14
12	4/12/04	1:25 PM	1.90	0.07	653	31	317	12
13	4/14/04	3:30 AM	2.58	0.12	614	171	2373	110
14	4/14/04	3:30 AM	2.28	0.11	614	171	2097	102
15	4/14/04	7:10 AM	2.66	0.07	646	155	2218	62
16	4/20/04	6:25 AM	2.18	0.06	761	55	645	17
17	4/20/04	10:25 AM	0.52	0.03	765	55	153	9
18	4/20/04	10:30 AM	0.52	0.03	765	55	153	9
19	4/21/04	12:05 PM	2.13	0.06	748	56	641	18
20	4/21/04	12:40 PM	2.30	0.07	735	60	742	24
21	4/22/04	2:30 PM	2.28	0.08	721	70	858	30
22	4/22/04	2:30 PM	2.41	0.09	721	70	907	34
23	4/22/04	9:40 PM	2.43	0.14	718	46	601	36
24	4/23/04	12:55 AM	2.35	0.08	714	40	506	18
25	5/14/04	4:15 PM	0.52	0.03	2002	0	1	0
26	5/14/04	4:18 PM	0.52	0.03	2002	0	1	0
27	5/14/04	5:40 PM	2.53	0.07	1992	1	12	0
28	5/14/04	7:20 PM	2.54	0.08	2689	1	18	1
29	5/15/04	7:30 PM	2.21	0.11	2689	35	416	21
30	5/15/04	7:31 PM	1.77	0.12	2689	35	333	22
31	5/15/04	11:30 PM	3.30	0.09	2665	26	462	12

Table 5-14. Discrete Sampling Data for Site EMIMI010

Data #	Date	Time	TN (mg/L)	TP (mg/L)	Conductivity (aes/cm)	Flow (cfs)	TN Load (lbs/d)	TP Load (lbs/d
1	03/03/04	8:45 AM	2.03	1.07	803	42	458	242
2	03/03/04	12:20 PM	0.52	0.03	815	40	111	6
3	03/03/04	1:20 PM	2.43	0.07	813	40	523	16
4	03/03/04	3:25 PM	2.30	0.08	815	45	557	20
5	03/04/04	1:25 PM	1.89	0.17	359	305	3099	271
6	03/04/04	1:26 PM	1.80	0.15	359	305	2951	252
7	03/04/04	5:40 PM	1.88	0.09	449	175	1769	89
8	04/12/04	10:55 AM	0.52	0.03	614	7.4	21	1
9	04/12/04	12:15 PM	1.58	0.09	554	7.8	66	4
10	04/12/04	2:00 PM	1.22	0.21	623	11	72	13
11	04/14/04	2:45 AM	2.14	0.33	381	181	2083	325
12	04/14/04	2:45 AM	2.25	0.35	381	181	2190	340
13	04/14/04	6:40 AM	1.99	0.18	423	138	1477	131
14	04/20/04	6:00 AM	2.00	0.12	729	13	140	8
15	04/20/04	9:15 AM	0.52	0.03	676	13	36	2
16	04/21/04	12:15 PM	2.03	0.18	684	14	153	14
17	04/21/04	12:40 PM	2.24	0.16	695	22	265	19
18	04/22/04	1:40 PM	1.89	0.14	519	30	305	22
19	04/22/04	1:40 PM	1.95	0.13	519	30	315	22
20	04/22/04	9:20 PM	2.24	0.16	540	40	482	34
21	04/23/04	12:25 AM	2.04	0.13	525	32	351	23
22	05/14/04	4:25 PM	0.52	0.03	703	8.7	24	1
23	05/14/04	4:35 PM	0.52	0.03	703	8.7	24	1
24	05/14/04	6:20 PM	2.40	0.36	705	12	155	23
25	05/14/04	8:35 PM	2.57	0.17	708	46	636	41
26	05/15/04	5:50 PM	0.66	0.17	695	110	388	100
27	05/15/04	5:51 PM	1.53	0.16	695	110	904	94
28	05/15/04	10:45 PM	2.05	0.15	501	65	717	51

The raw data sets given in the Tables above were partitioned into two distinct sets namely the training data set and the validation data set. The training data sets (comprising of 80% of the total data) were used in the development of the inductive models and the validation data sets (comprising of 20% of the total data) were used in validating the inductive models.

5.3.2.2.2.1 Regression Models

Linear multiple regression inductive models were developed for predicting total nitrogen and total phosphorus loads based on the daily stream flow and specific conductance measurements collected at each of the three sites discussed above. The general form of the multiple linear regression models is given as follows:

$$TN \text{ or } TP = a_0 + a_1 Q + a_2 C \qquad (5\text{-}7)$$

where a_0 through a_n are regression coefficients, Q (daily stream flow) and C (conductivity) are the independent variables in the regression model, and *TP or TN* loads (total nitrogen or total phosphorus) is the dependent variable to be predicted by the model. The regression models are given as follows in Equations 5-8 through 5-13 and Figures 5-25 through 5-36.

$$(TN)_{EMUMU001} = -424.30 + 16.34Q + 0.16C \qquad (5\text{-}8)$$

$$(TP)_{EMUMU001} = -19.77 + 0.56Q - 0.008C \qquad (5\text{-}9)$$

$$(TN)_{EMIMI010} = 373.27 + 9.56Q - 0.54C \qquad (5\text{-}10)$$

$$(TP)_{EMIMI010} = 15.77 + 1.05Q - 0.0138C \qquad (5\text{-}11)$$

$$(TN)_{ESFS006} = 825.71 + 10.74Q - 1.12C \qquad (5\text{-}12)$$

$$(TP)_{ESFSF006} = 503.21 + 1.38Q - 0.78C \qquad (5\text{-}13)$$

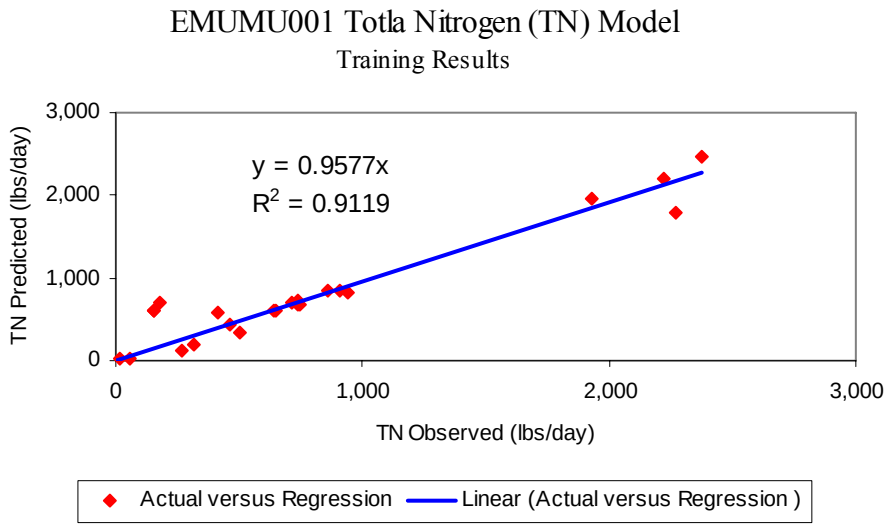


Figure 5-25. Regression-based Total Nitrogen Model for Site EMUMU001 (Model Training)

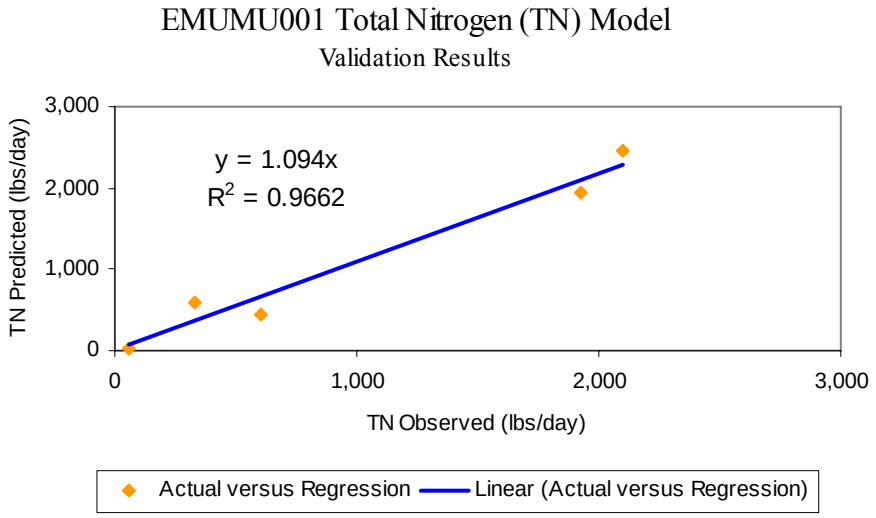


Figure 5-26. Regression-based Total Nitrogen Model for Site EMUMU001 (Model Validation)

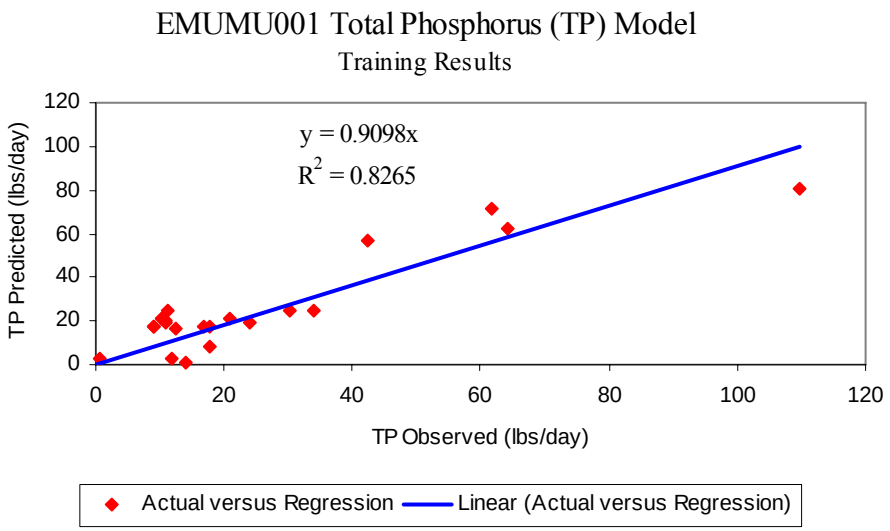


Figure 5-27. Regression-based Total Phosphorus Model for Site EMUMU001 (Model Training)

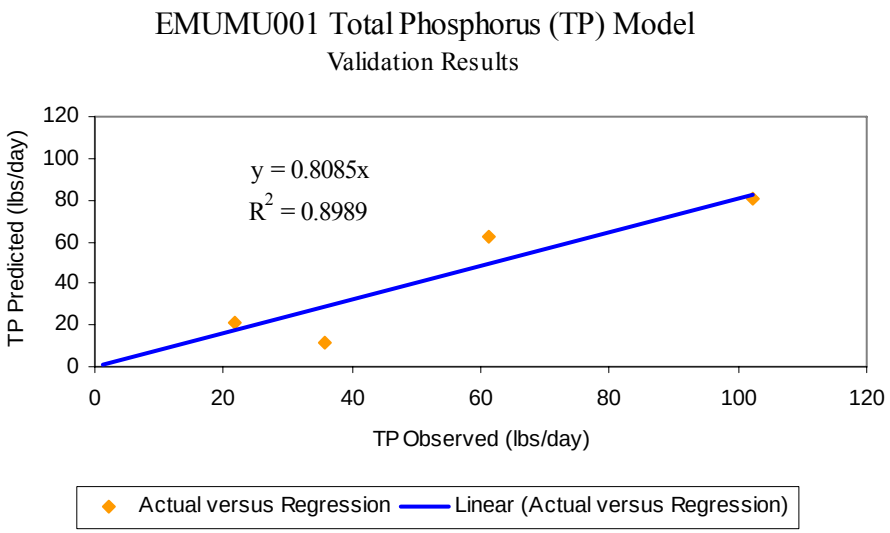


Figure 5-28. Regression-based Total Phosphorus Model for Site EMUMU001 (Model Validation)

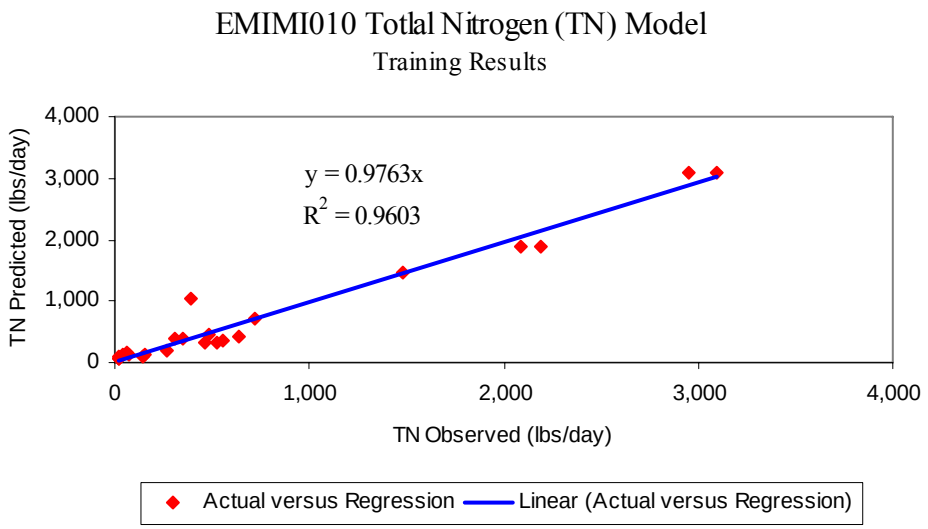


Figure 5-29. Regression-based Total Nitrogen Model for Site EMIMI010 (Model Training)

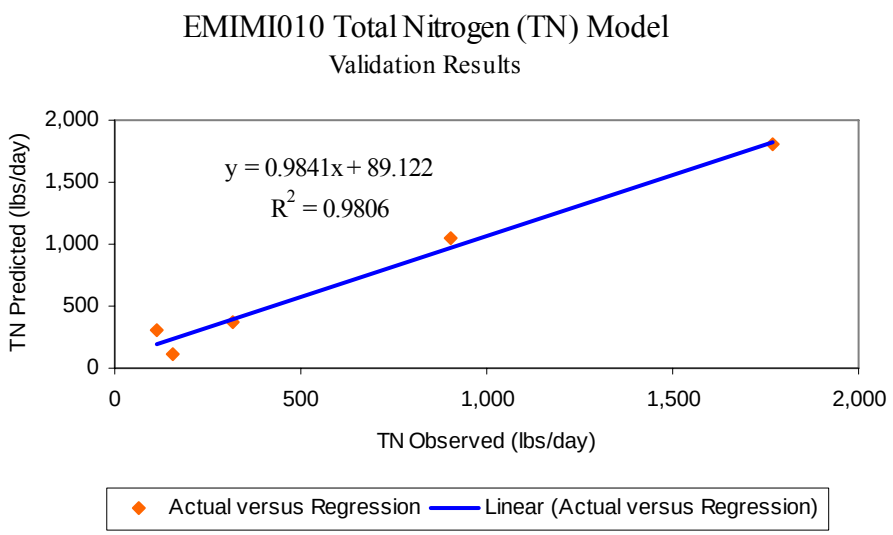


Figure 5-30. Regression-based Total Nitrogen Model for Site EMIMI010 (Model Validation)

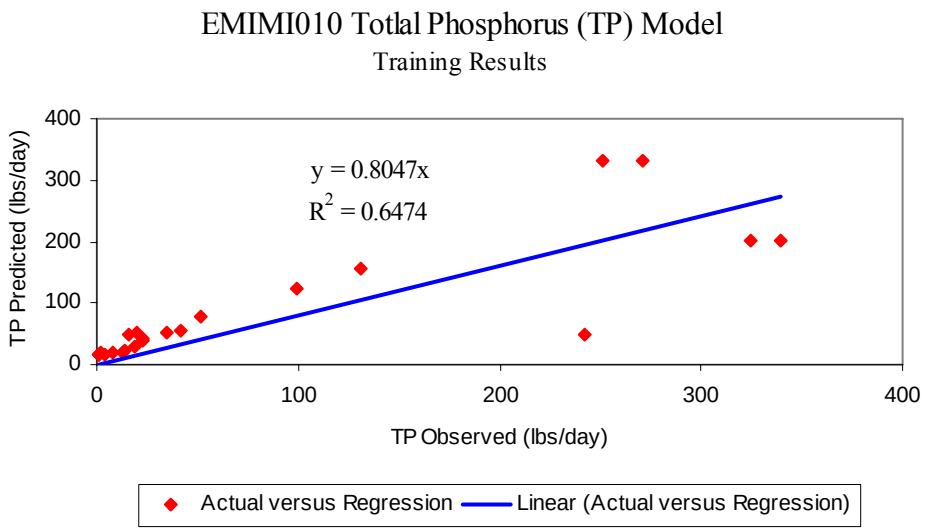


Figure 5-31. Regression-based Total Phosphorus Model for Site EMIMI010 (Model Training)

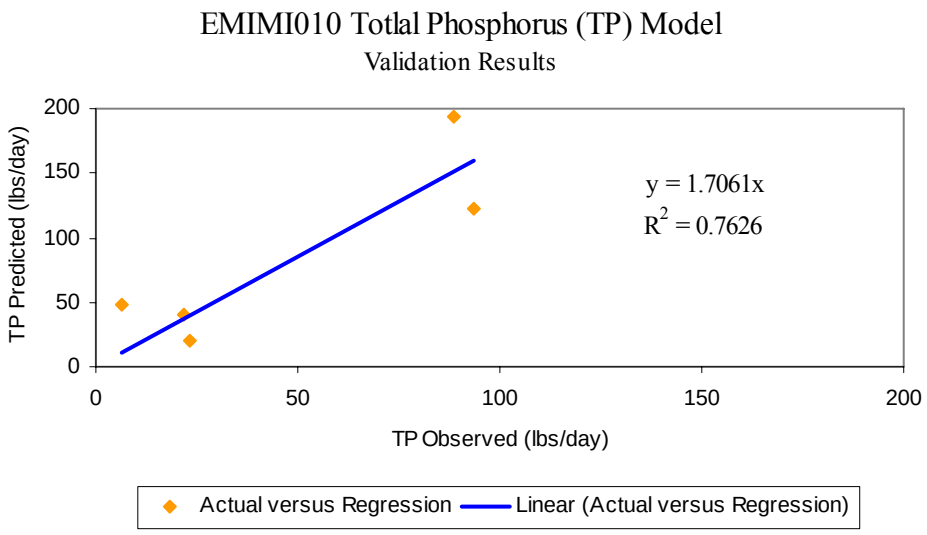


Figure 5-32. Regression-based Total Phosphorus Model for Site EMIMI010 (Model Validation)

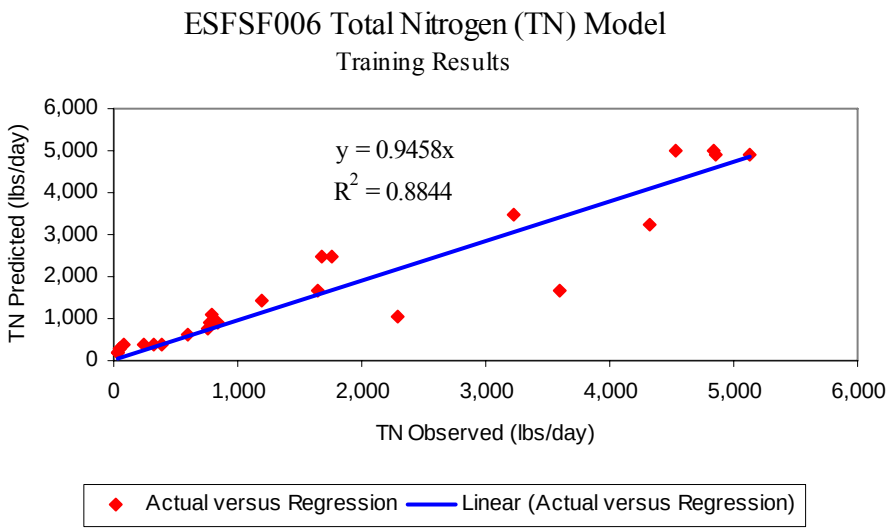


Figure 5-33. Regression-based Total Nitrogen Model for Site ESFSF006 (Model Training)

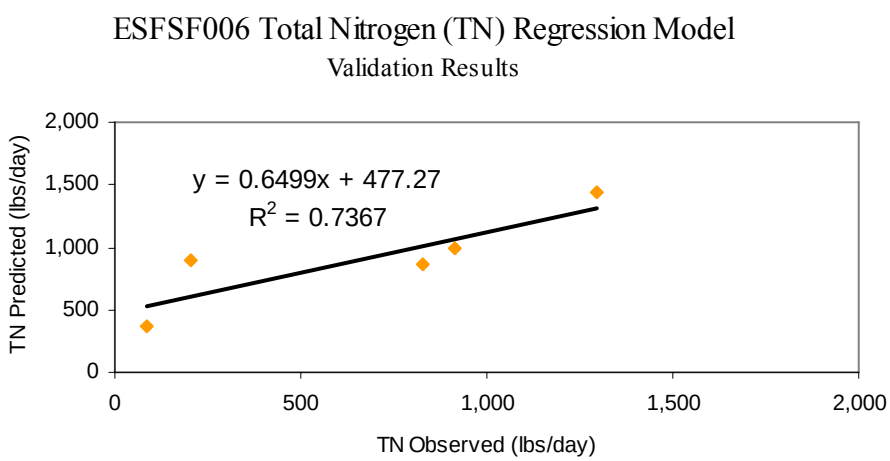


Figure 5-34. Regression-based Total Nitrogen Model for Site ESFSF006 (Model Validation)

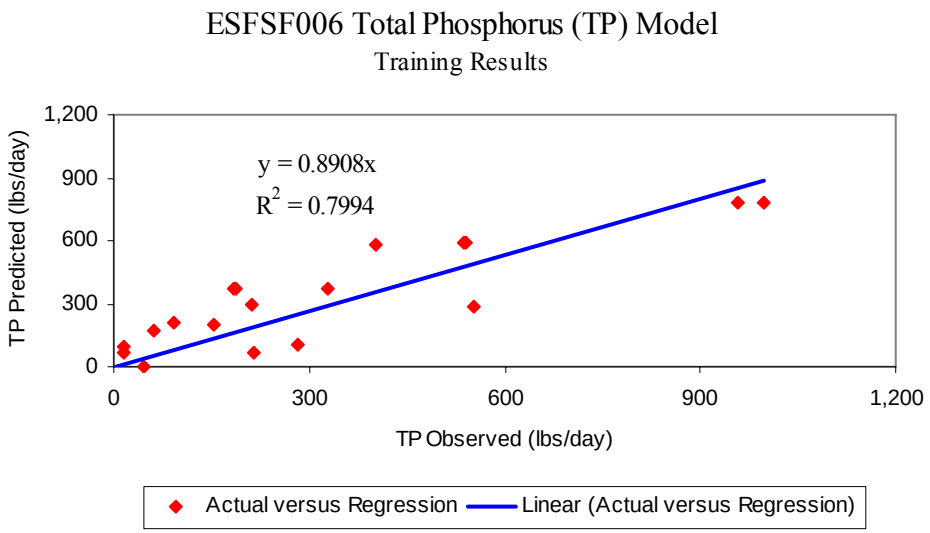


Figure 5-35. Regression-based Total Phosphorus Model for Site ESFSF006 (Model Training)

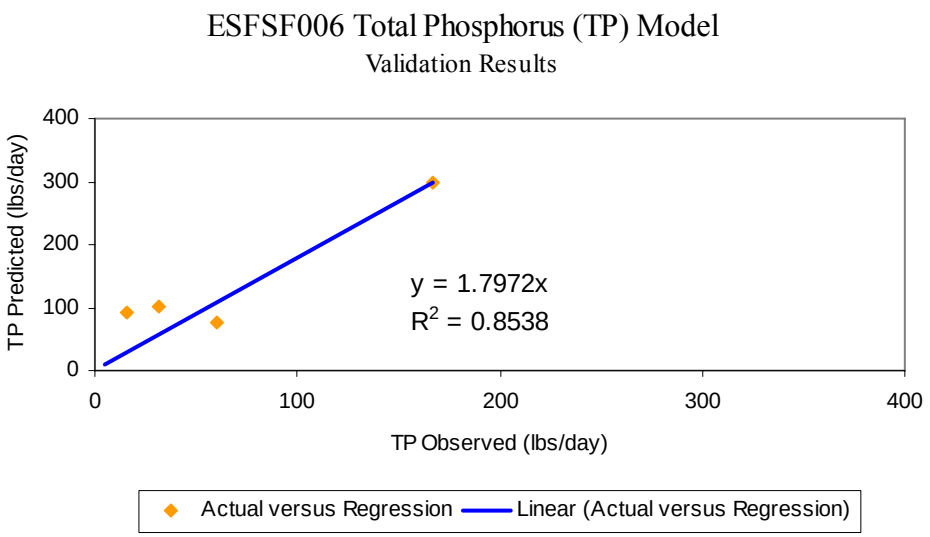


Figure 5-36. Regression-based Total Phosphorus Model for Site ESFSF006 (Model Validation)

5.3.2.2.2.2 ANN Models

The popular multi layer feed-forward back propagation neural networks were used in developing nutrient inductive models. The model structure included one input layer, one hidden layer, and a corresponding output layer. The input layer consists of two input nodes representing daily stream flow (Q) and conductivity (C) whereas the output layer consist of one node representing the target total nitrogen or total phosphorus load (TN or TP). The number of hidden nodes in the hidden layer (H) was varied in the model development, starting with two nodes and going up to a maximum of six nodes. A general schematic of the ANN structure used in developing the nutrient inductive models is given below in Figure 5-37.

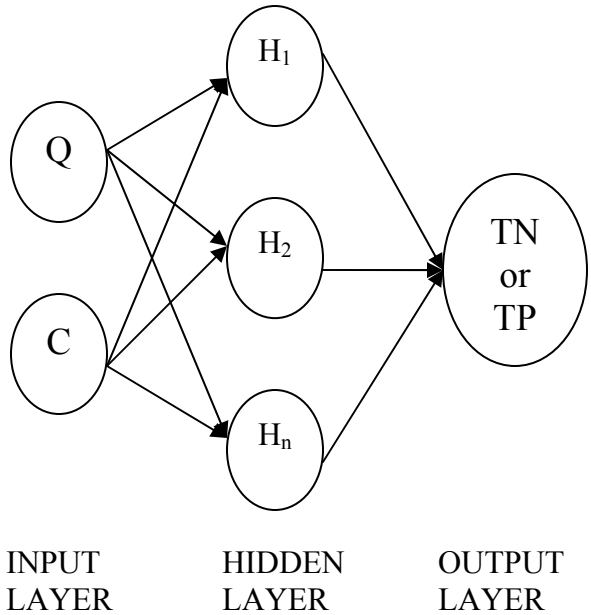


Figure 5-37. Neural Network Structure for Inductive Nutrient Models

The ANN network architecture was varied by trying different number of hidden nodes in the hidden layer and varying the learning rate and momentum rate parameters. In the majority of evaluations, the most optimal results were obtained by using two hidden nodes in the hidden layer. The ANN structure used for nutrient modeling used a logistic sigmoid function of the form given as:

$$f(x) = \frac{1}{1+e^{-x}} \qquad (5\text{-}14)$$

Figures 5-38 through 5-49 gives the results of the ANN-based nutrient models developed for each of the three sites.

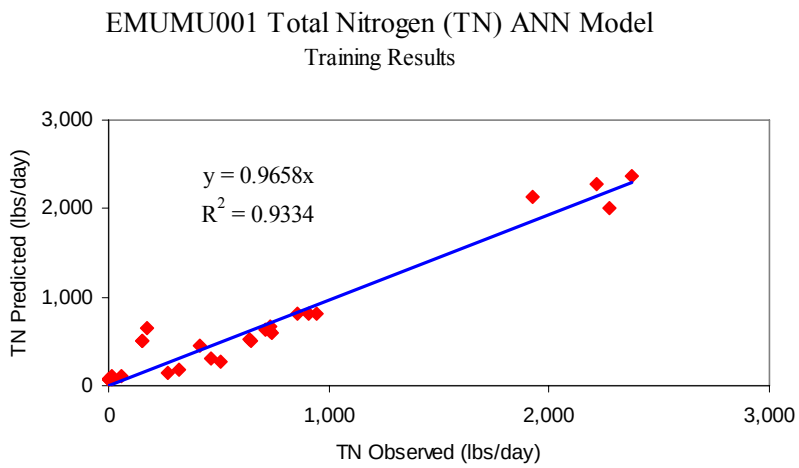


Figure 5-38. ANN-based Total Nitrogen Model for Site EMUMU001 (Model Training)

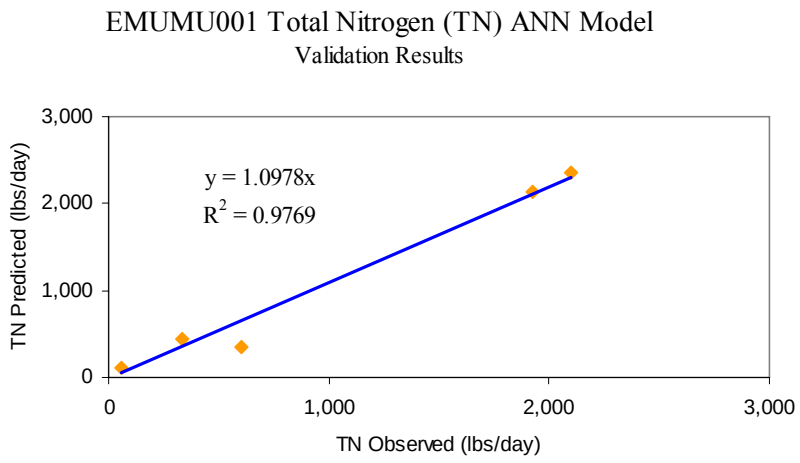


Figure 5-39. ANN-based Total Nitrogen Model for Site EMUMU001 (Model Validation)

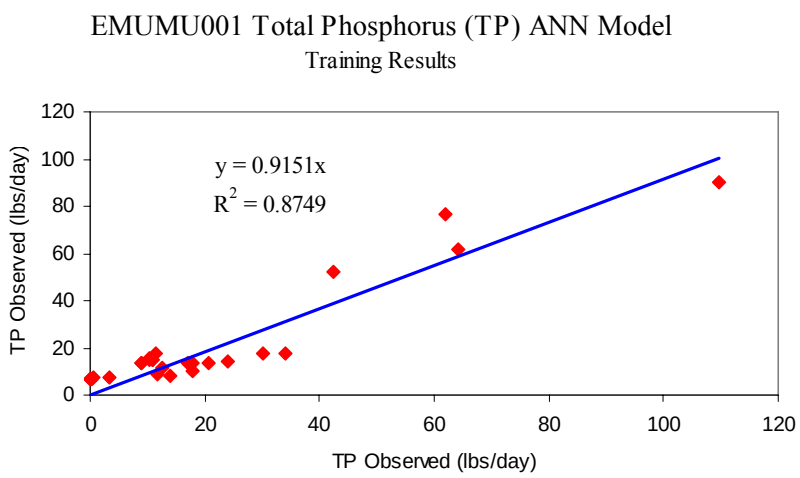


Figure 5-40. ANN-based Total Phosphorus Model for Site EMUMU001 (Model Training)

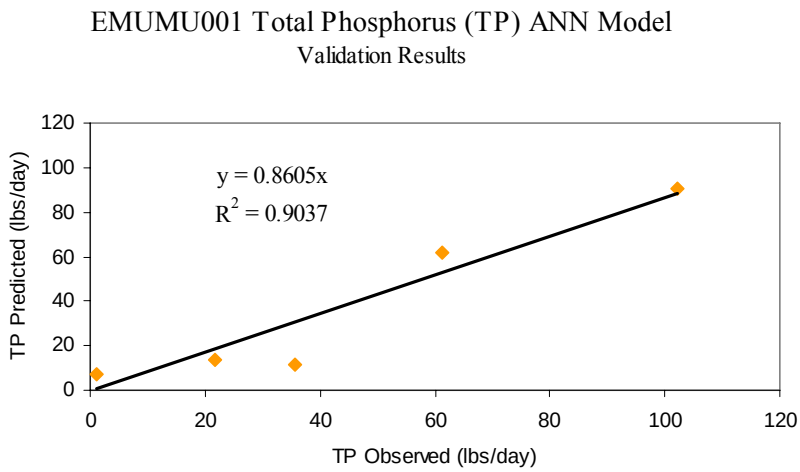


Figure 5-41. ANN-based Total Phosphorus Model for Site EMUMU001 (Model Validation)

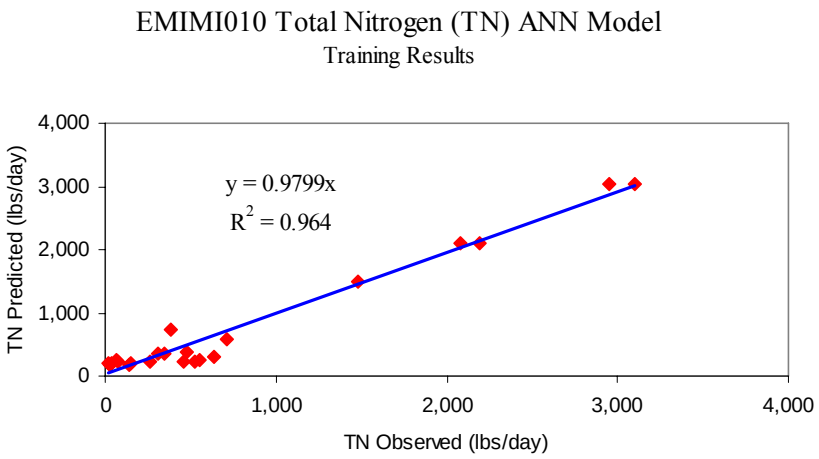


Figure 5-42. ANN-based Total Nitrogen Model for Site EMIMI010 (Model Training)

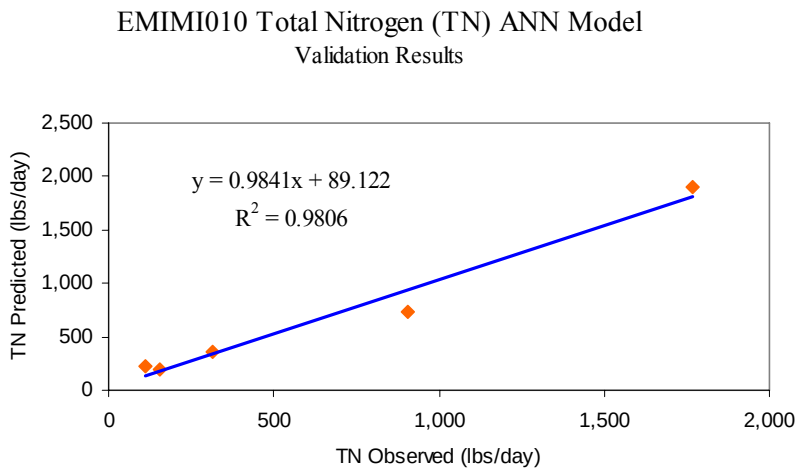


Figure 5-43. ANN-based Total Nitrogen Model for Site EMIMI010 (Model Validation)

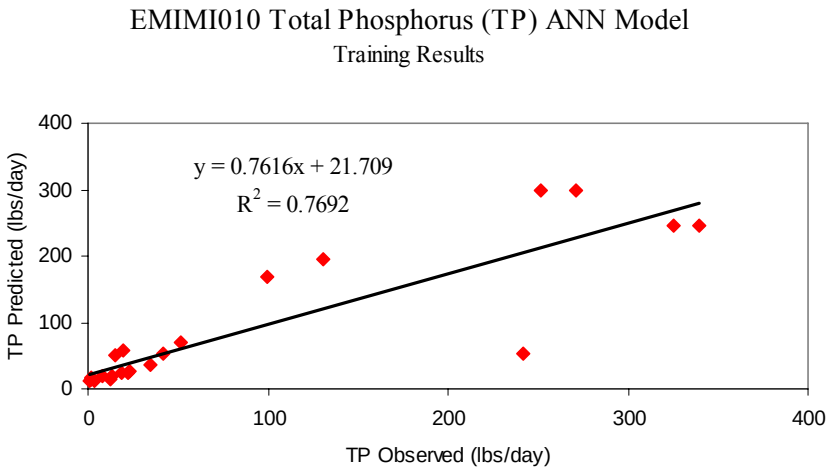


Figure 5-44. ANN-based Total Phosphorus Model for Site EMIMI010 (Model Training)

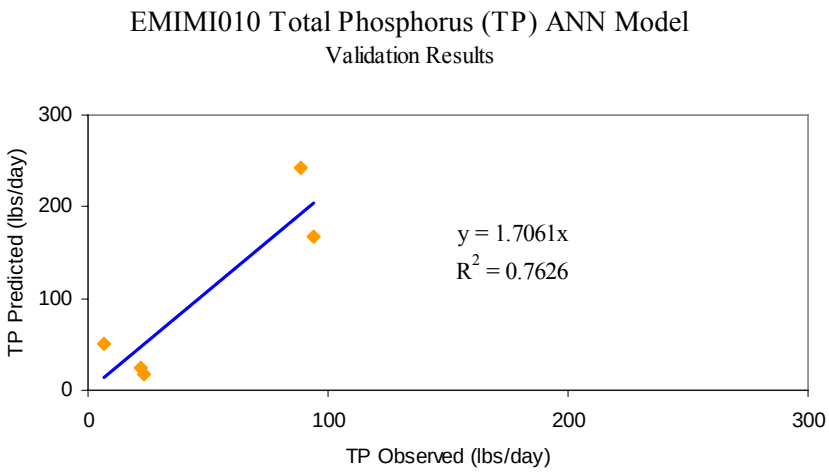


Figure 5-45. ANN-based Total Phosphorus Model for Site EMIMI010 (Model Validation)

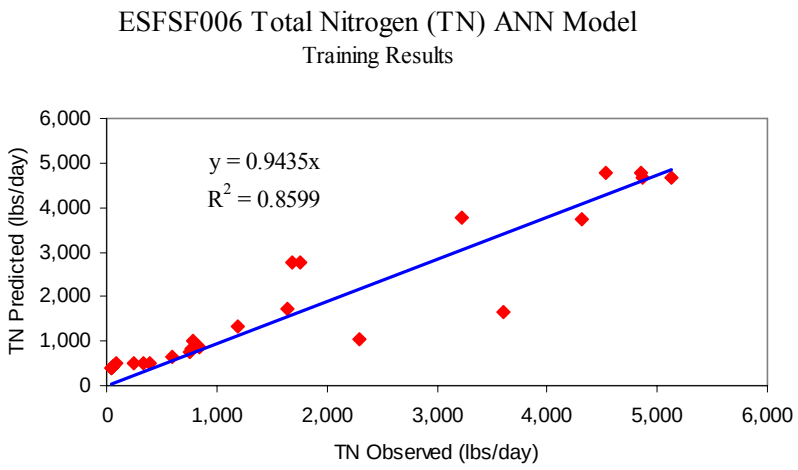


Figure 5-46. ANN-based Total Nitrogen Model for Site ESFSF006 (Model Training)

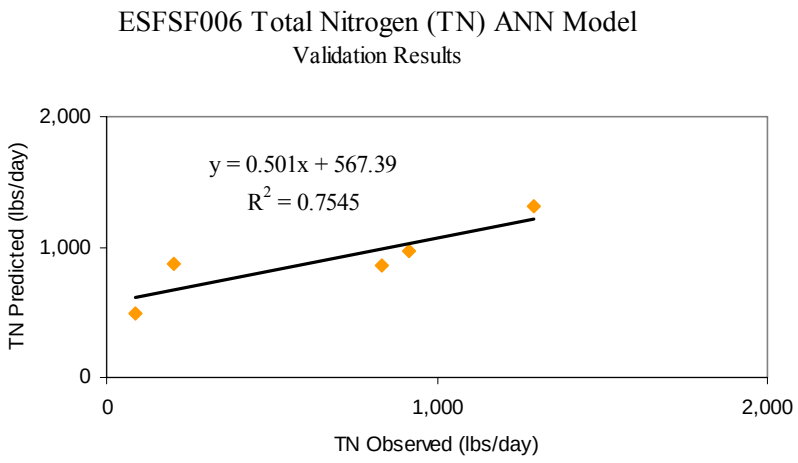


Figure 5-47. ANN-based Total Nitrogen Model for Site ESFSF006 (Model Validation)

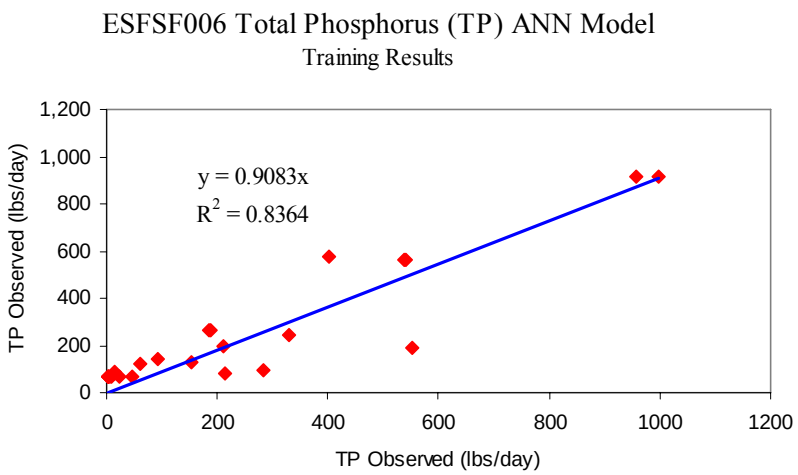


Figure 5-48. ANN-based Total Phosphorus Model for Site ESFSF006 (Model Training)

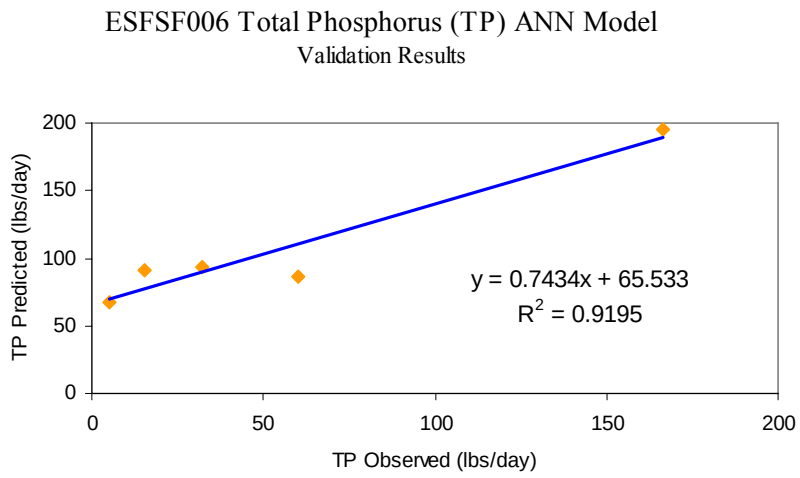


Figure 5-49. ANN-based Total Phosphorus Model for Site ESFSF006 (Model Validation)

5.3.2.2.2.3 FFSGA Models

The FFSGA approach of developing empirical equations for a response function was investigated for one of the sampling site (ESFSF006 on South Fork) to illustrate the utility of this approach. Five different fixed functional forms were formulated to represent the expressions for total nitrogen and total phosphorus as given in Figure 5-50 (these represent the general pre-defined form of the empirical expressions sought), each being some combination of elementary sub-functions of the independent variables in the data set. These functional forms also consist of coefficients that act as weighting factors for the elementary sub-functions of the decision variables (independent variables). The two independent variables consists of the daily stream flow (Q) and the specific conductance (C). Table 5-15 gives a list of a sample of 15 different sub-functions for each of the independent variables (model inputs) that are available for selection by the FFSGA model. Table 5-16 gives the mathematical operators that are available for selection by the FFSGA model.

Functional Form #1 = {C_1 operator_1 [function_1 (Q) operator_2 function_2 (C)]} operator_3 {C_2 operator_4 [function_3 (Q) operator_5 function_4 (C)]}

Functional Form #2 = {C_1 * [function_1 (Q) operator_1 function_2 (C)]} operator_2 {C_2 * [function_3 (Q) operator_4 function_4 (C)]}

Functional Form #3 = {C_1 * function_1 (Q) * function_2 (C)} operator_1 {C_2 * function_3 (Q) * function_4 (C)}

Functional Form #4 = {C_1 * function_1 (Q)} operator_1 {C_2 * function_2 (C)}

Functional Form #5 = {[C_1 * function_1 (Q)] operator_1 [C_2 * function_2 (C)]} operator_2 {C_3 * function_3 (Q) * function_4 (C)}

Figure 5-50. Pre-defined FFSGA Functional Forms for Inductive Nutrient Models

Table 5-15. List of functions for Flow (Q) and Conductivity (C)

Function #	Function f (Q) or Function f (C)
1	1
2	Q or C or Sqrt(Q) or Sqrt(C)
3	1/Q or 1/(C)
4	Exp (Q) or Exp (C)
5	Log_e (Q) or Log_e (C)
6	Log_{10} (Q) or Log_{10} (C)
7	Exp (1/Q) or Exp (1/ C)
8	Log_e (1/Q) or Log_e (1/ C)
9	Log_{10} (1/Q) or Log_{10} (1/ C)
10	Q*Exp(Q) or C *Exp(C)
11	Q* Log_e (Q) or C *Log_e (C)
12	Q*Log_{10} (Q) or C *Log_{10} (T)
13	(1/Q)*Exp(Q) or (1/ C)*Exp(C)
14	(1/Q)* Log_e (Q) or (1/ C)*Log_e (C)
15	(1/Q)*Log_{10} (Q) or (1/ C)*Log_{10} (C)

Table 5-16. List of Operators in the General Functional Forms

Operator #	Operator
1	+
2	-
3	*
4	/
5	^

The FFSGA model evaluates each of the five functional forms (Figure 5-50) individually. The search for the optimal expression is carried out using the FFSGA model as discussed in Chapter 4. At the termination of specified generations, the functional form that has the highest fitness value is the optimal structure of the explicit expression sought in the search process. Finally, the coefficients of the functional form are obtained by applying least squares optimization to the optimal form obtained from the GA process. Equations 5-15 and 5-16 give the optimal expressions resulting from the FFSGA approach for total nitrogen and total phosphorus loads. The results of the FFSGA-based nutrient models using these equations in predicting the total nitrogen and total phosphorus loads for the South Fork of Beargrass Creek sampling site (ESFSF006) are given in Figures 5-51 through 5-54.

$$TN = 5.32 * \left[\frac{Q * \log_{10} Q}{\log_{10}\left(\frac{1}{C}\right)} \right] * (-8.23) - \left[Ln\left(\frac{1}{Q}\right) - \frac{1}{C} * Ln\left(\frac{1}{C}\right) \right] \quad (5\text{-}15)$$

$$TP = -69.39 * \left[Q * Ln\left(\frac{1}{Q}\right) - \exp\left(\frac{1}{C}\right) \right] * \left[\frac{74.81}{Ln(Q) * (C * Ln(C))} \right] \quad (5\text{-}16)$$

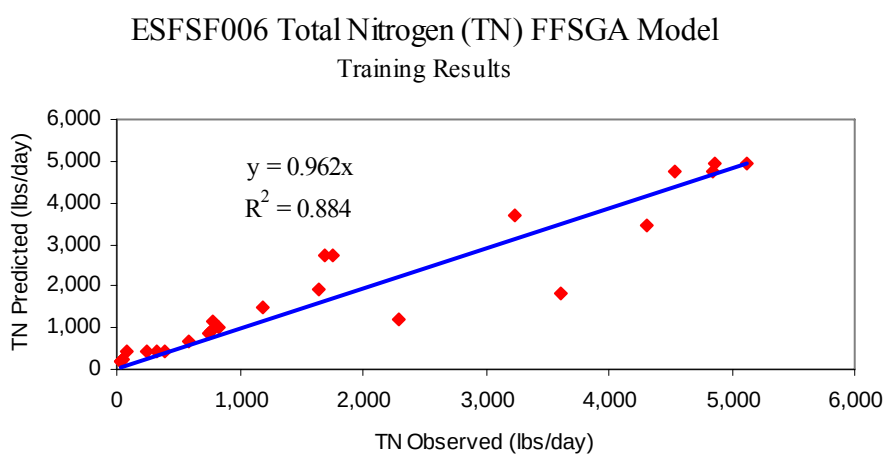


Figure 5-51. FFSGA-based Total Nitrogen Model for Site ESFSF006 (Model Training)

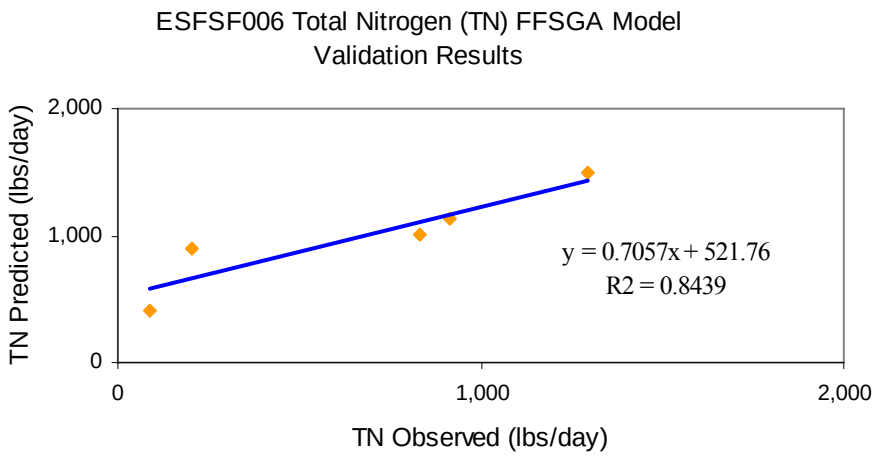


Figure 5-52. FFSGA-based Total Nitrogen Model for Site ESFSF006 (Model Validation)

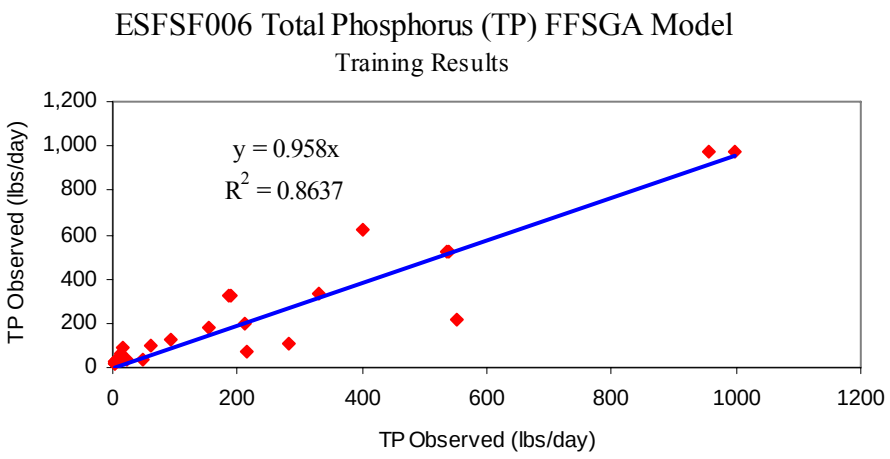


Figure 5-53. FFSGA-based Total Phosphorus Model for Site ESFSF006 (Model Training)

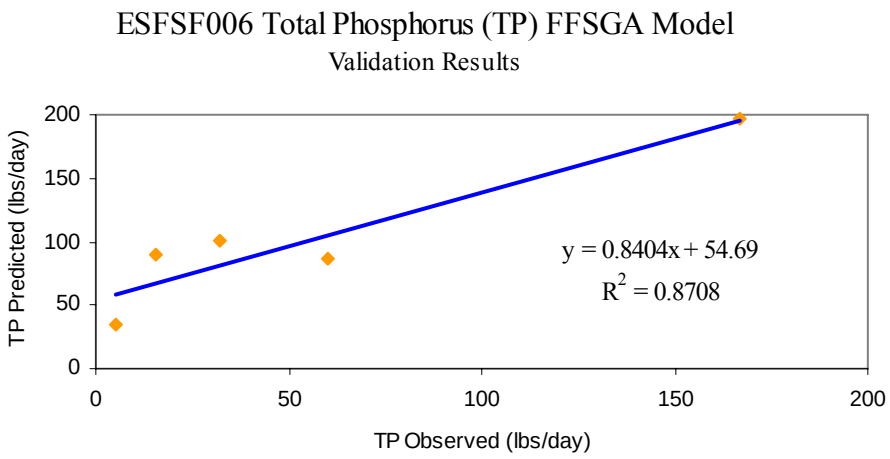


Figure 5-54. FFSGA-based Total Phosphorus Model for Site ESFSF006 (Model Validation)

5.3.2.2.3 Summary of Results for Nutrient Models

The three types of inductive models (regression, ANNs, and FFSGA) for predicting nutrient loads in the Beargrass Creek watershed shows that there is a strong correlation between stream flows and nutrient loads. All three types of models performed equally well as demonstrated by the plots given above. To demonstrate the relative performance of these three methods, Tables 5-17 through 5-20 gives the different measures of performance for the three methods at one of the three sites. The South Fork site ESFSF006 was chosen for comparison since all three types of models were developed for this site. The measure of performance reported includes the coefficient of determination (R^2), mean square error (MSE), and average absolute error of prediction in both training and validation.

Table 5-17. Results Summary of Total Nitrogen (TN) Inductive Models in Training

Data Set Description Model Performance	Regression (Training)	ANN (Training)	FFSGA (Training)
# of Data	25	25	25
Average Absolute Error	358	417	383
Max Absolute Error	1,930	1,959	1,789
Mean Square Error (MSE)	334,737	313,399	321,107
Coefficient of Determination (R^2)	0.88	0.86	0.88

Table 5-18. Results Summary of Total Nitrogen (TN) Inductive Models in Validation

Data Set Description Model Performance	Regression (Validation)	ANN (Validation)	FFSGA (Validation)
# of Data	5	5	5
Average Absolute Error	244	235	210
Max Absolute Error	689	669	502
Mean Square Error (MSE)	116,042	123,495	112,052
Coefficient of Determination (R^2)	0.74	0.75	0.83

Table 5-19. Results Summary of Total Phosphorus (TP) Inductive Models in Training

Data Set Description Model Performance	Regression (Training)	ANN (Training)	FFSGA (Training)
# of Data	25	25	25
Average Absolute Error	95	80	64
Max Absolute Error	265	366	338
Mean Square Error (MSE)	14,622	10,203	10,612
Coefficient of Determination (R^2)	0.80	0.84	0.86

Table 5-20. Results Summary of Total Phosphorus (TP) Inductive Models in Validation

Data Set Description Model Performance	Regression (Validation)	ANN (Validation)	FFSGA (Validation)
# of Data	5	5	5
Average Absolute Error	62	51	46
Max Absolute Error	131	76	75
Mean Square Error (MSE)	5,665	3,012	2,540
Coefficient of Determination (R^2)	0.85	0.92	0.87

It is worth mentioning to note that the FFSGA method performed better than regression and ANN in the Total Nitrogen validation model in all four measures of performance. The FFSGA model also performed better in three of the four measures of performance (MSE, maximum absolute error, and average absolute error) in the Total Phosphorus validation model. FFSGA has the ability to perform well under data scarce situations as is the case in this particular application. On the contrary, ANN is particularly suited to applications where large amount of data is available for model training.

5.3.2.3 Explicit Inductive Models for Dissolved Oxygen (DO)

Explicit inductive models were developed to predict dissolved oxygen in the receiving waters of the Beargrass Creek watershed. These are described as follows.

5.3.2.3.1 Study Area

The Beargrass Creek watershed has multiple stream segments that are listed on the State's 303(d) list for violating the DO standards as shown in Figure 5-23. Per Kentucky Water Quality Standards, the dissolved oxygen criterion for aquatic life is 5.0 mg/L (daily average) and 4.0 mg/L (instantaneous minimum) (Kentucky Administrative Regulations Title 401, Chapter 5, Water Quality). These include all of the South Fork and the lower reaches of the Middle Fork. A comprehensive water quality sampling program is in place for this watershed that includes both continuous water quality monitoring and discrete sampling for key parameters. The continuous sampling include DO meters that samples data every 15 minutes. Data collected for this watershed was used to develop explicit inductive models for dissolved oxygen.

5.3.2.3.2 Dissolved Oxygen

Dissolved oxygen refers to the volume of oxygen that is contained in a water column (Radwan et al. 2003). Oxygen enters a water body by photosynthesis of aquatic plants and by the transfer of oxygen across the air-water interface. Dissolved oxygen (DO) is vital to fish, shellfish and other aquatic life living in a given water body. These organisms

respire using the oxygen dissolved in water and are essentially suffocated when there is not enough oxygen available. Low DO is frequently caused by excess nutrients, which can consume oxygen as they are chemically transformed or can cause algal blooms which then die-off and consume oxygen as they decompose. The ability of a stream to maintain an acceptable dissolved oxygen (DO) concentration is an important consideration in determining its capacity to assimilate wastewater discharges. DO is used in the microbial oxidation of organic and certain inorganic matter present in wastewater. Oxygen supplied principally by re-aeration from the atmosphere will replace any DO lost through oxidation processes. If, however, the rate of oxygen use exceeds the rate of re-aeration, the DO concentration may decrease below minimum allowable standards (Thomann and Mueller, 1987).

Sources and Sinks of DO

To develop a water quality model for simulating DO dynamics in a stream, all significant factors affecting the DO process should be clearly understood and considered in the modeling. In a typical water body, the sources of DO are (Thomann and Mueller, 1987):

1. Re-aeration from the atmosphere.
2. Photosynthetic oxygen production.
3. DO in incoming tributaries.

Similarly, the sinks of DO are listed as follows:

1. Oxidation of carbonaceous waste material.
2. Oxidation of nitrogenous waste material.
3. Oxygen demand of sediments of water body.
4. Use of oxygen for respiration by aquatic plants.

Environmental Impacts of Dissolved Oxygen

The introduction of excess organic matter or oxygen consuming material may result in a depletion of oxygen in a water body, mainly during warm and stagnant conditions in

which water mixing is minimal (Radwan et al. 2003). Gower (1980) reported that exposure to less than 30% saturation (less than 2 mg/L) for one to four days may kill most of the biota in a system. Also, prolonged exposure to low DO levels (less than 5 mg/L) may not directly kill an organism, but can increase its susceptibility to many other environmental stresses.

Inductive models are data-based models and in-depth knowledge of the process being modeled is often not required. However, if available, knowledge of the process modeled can facilitate model development by providing insights into the factors affecting the process. To develop an inductive or empirical model for simulating DO in a water body, observed data collected in the field is used that includes DO and other parameters that can affect the DO dynamics in the water body. These can include parameters such as nutrients (total nitrogen and total phosphorus), stream flows, and temperature. The data used in the development of the DO inductive models was obtained from MSD personnel involved in the data collection and management of the Beargrass Creel watershed. The following sub-sections will describe the development of inductive DO receiving water models for the Beargrass Creek watershed in Louisville, Kentucky.

5.3.2.3.3 Structure of Inductive DO Receiving Water Model

An ANN-based inductive receiving water model was constructed for simulating DO in the Beargrass Creek watershed (Figure 5-23). The inductive model relates the DO to stream flows (Q), nutrients (TN and TP) and temperature (T). A two-step approach of inductive model development was employed that included 1) a source-load inductive model to simulate nutrients as a function of flow and conductivity, and 2) a receiving water inductive model that relates the stream flows, nutrients, and temperature to DO in the stream as shown in Figure 5-55 and 5-56. The source load model was constructed using three different techniques namely regression method, ANNs, and FFSGA. The receiving water model was constructed using ANN due to its ability to work with large sets of data.

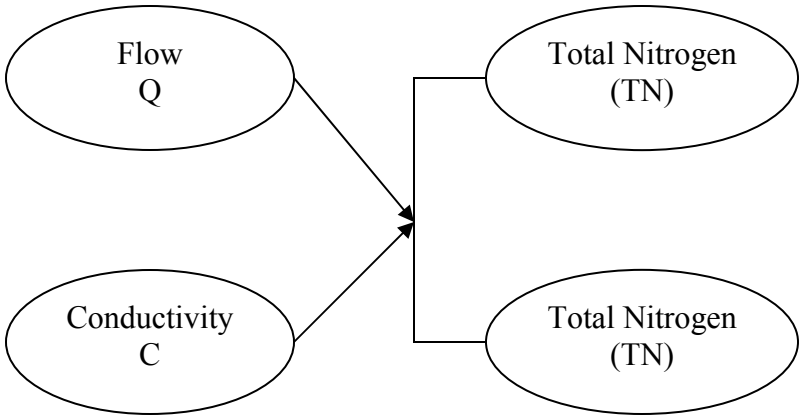


Figure 5-55. Source-load ANN Model for Nutrients

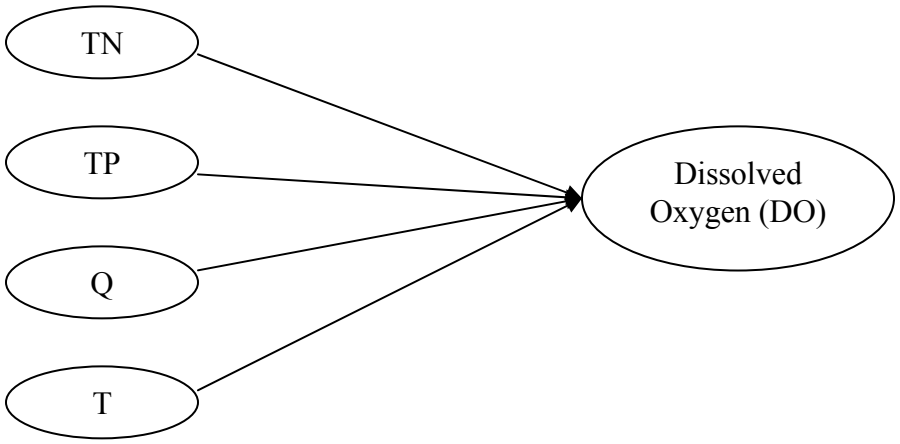


Figure 5-56. Receiving Water ANN Model for Dissolved Oxygen

5.3.2.3.4 Development of DO Inductive Model

The nutrient inductive models for predicting TN and TP loads constitute the first phase (Figure 5-55) in the two-phase process for DO inductive receiving water model as outlined above and these were described in the previous section. The second phase (Figure 5-56) consists of using the nutrient loads (computed using the nutrient inductive models) as inputs to a DO inductive receiving water model along with other related

parameters such as temperature and streams flow. The target output of such a model will be the measured DO concentration obtained from the continuous DO meters at the point of interest in the watershed. For these models to be effective, it is important that in addition to be accurate in predicting DO, these models also establishes a reasonably accurate cause-and-effect relationship between inputs and outputs. Once such a relationship is established by these inductive models, they can be used in evaluating different management strategies leading to load reductions in nutrient loads in contributing sub-watersheds.

The DO inductive receiving water model is based on the ANN inductive modeling technique. Two different categories of DO models were investigated and these include 1) one that uses an hourly time step, and 2) one that uses a daily time step. The DO continuous monitoring data is in 15-minute intervals and is aggregated into hourly and daily intervals for use in the two categories of ANN inductive models.

5.3.2.3.4.1 ANN-based Hourly-DO Inductive Model

In the hourly DO inductive model, the inputs to the model consists of hourly stream flow, temperature, conductivity, total nitrogen load, and total phosphorus load. The output consists of the target hourly DO concentration at the confluence of all contributing tributaries in the watershed (Site ESFSF013). Figure 5-57 shows the location of this site along with the location of the three sites used for development of nutrient models as described in the previous section. The stream flow data is obtained from the USGS gage stations in each of the tributary sub-watersheds as shown in Figure 5-57. Such a receiving water DO model can be used to determine total nutrients load reduction strategies needed to bring the DO at site ESFSF013 in compliance with regulatory limits.

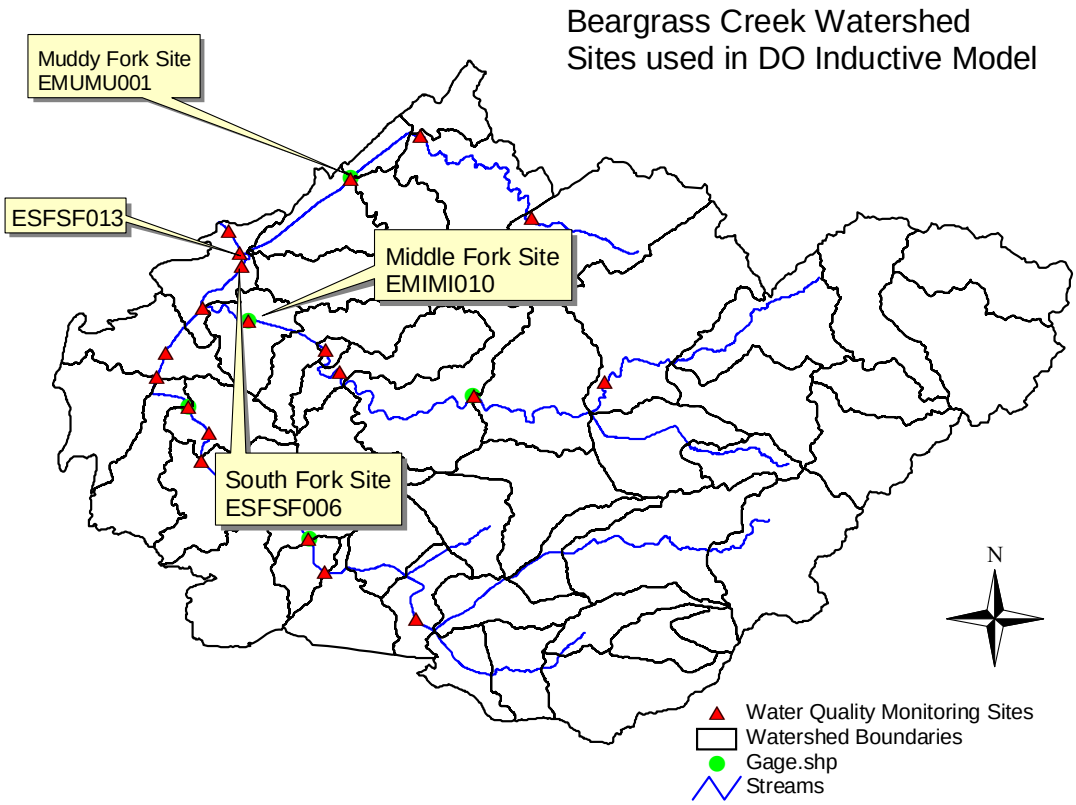


Figure 5-57. Sites used in the DO Inductive Models

The popular multi layer feed-forward back propagation neural networks were used in developing the hourly inductive model for DO. The model structure included one input layer, one hidden layer, and a corresponding output layer. The input layer consists of five input nodes representing daily stream flow (Q), conductivity (C), temperature (T), total nitrogen load (TN), and total phosphorus (TP). The output layer consists of one node representing the target DO concentration (DO). The number of hidden nodes (H) in the hidden layer was varied in the model development, starting with five nodes and going up to a maximum of twelve nodes. A general schematic of the ANN model structure used in developing the hourly DO inductive model is given below in Figure 5-58.

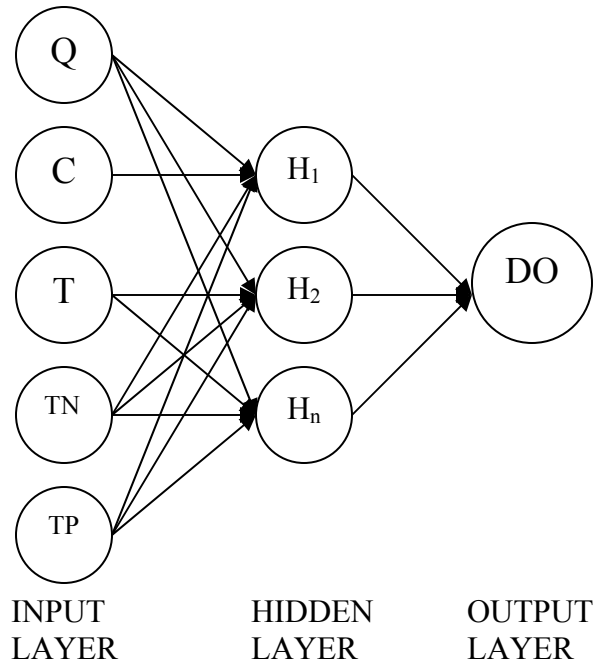


Figure 5-58. Neural Network Structure for Hourly Inductive DO Model

The ANN network architecture was varied by trying different number of hidden nodes in the hidden layer and varying the learning rate and momentum rate parameters. In the majority of evaluations, the most optimal results were obtained by using five hidden nodes in the hidden layer. The ANN structure used for fecal modeling used a logistic sigmoid function of the form given as:

$$f(x) = \frac{1}{1+e^{-x}} \qquad (5\text{-}17)$$

The data used in the model development included data collected for the period January 1, 2004 through November 30, 2004. The hourly data set (comprising of a total of 4,118 data points) was partitioned into training and a validation data set. A total of 3,600 data points were used for model training and the remaining 518 data points were used for

model validation. Figure 5-59 and 5-60 below shows the actual versus predicted DO from the ANN model in training as well as validation.

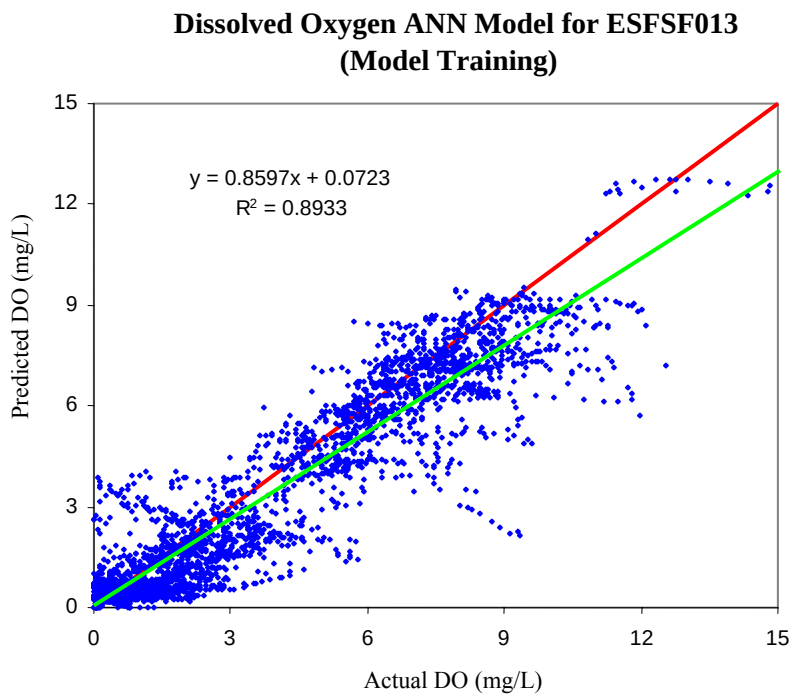


Figure 5-59. Dissolved Oxygen ANN Model (Training Results)

The line in red above is a 45-degree line and the green line is the linear trend line for the data. The model performs very well in prediction as shown by the high coefficient of determination (0.89). The model performs equally well in validation and has a coefficient of determination of 0.87 as shown in Figure 5-60 below.

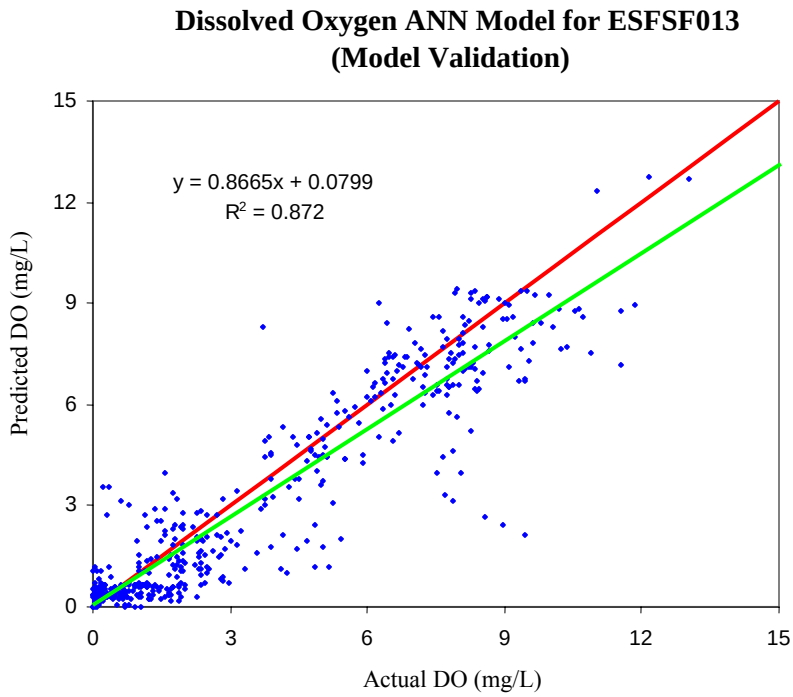


Figure 5-60. Dissolved Oxygen ANN Model (Validation Results)

Table 5-21 below gives the measures of performance for the DO model in training and validation.

Table 5-21. Measure of Performance of the Dissolved Oxygen ANN Model

Model Type	Coefficient of Determination ($R^{2)}$	Mean Square Error (MSE)	Average Absolute Error	Maximum Absolute Error
Training	0.89	1.31	0.78	7.22
Validation	0.87	1.58	0.84	7.33

An error analysis was carried out for the ANN model in training and validation to demonstrate that the error is randomly distributed and there is no significant trend followed. The error graphs for the ANN-based hourly DO models in both training and validation are shown in Figures 5-61 and 5-62 below.

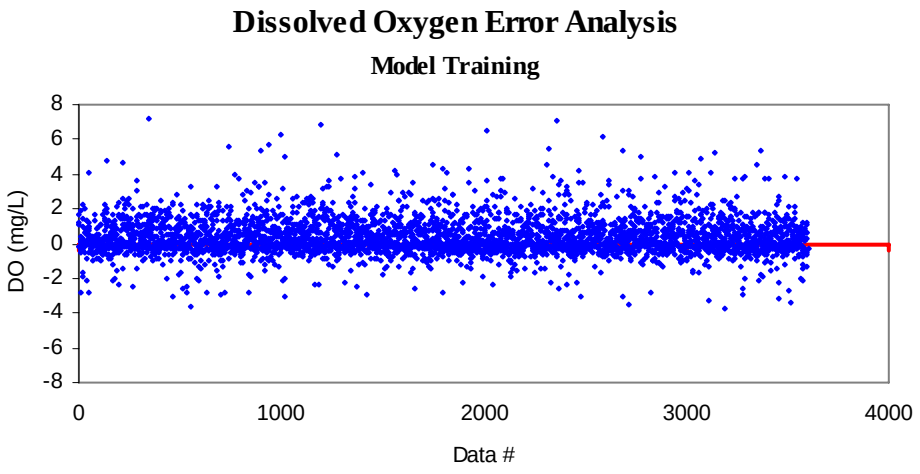


Figure 5-61. Dissolved Oxygen ANN Training Model Error Analysis

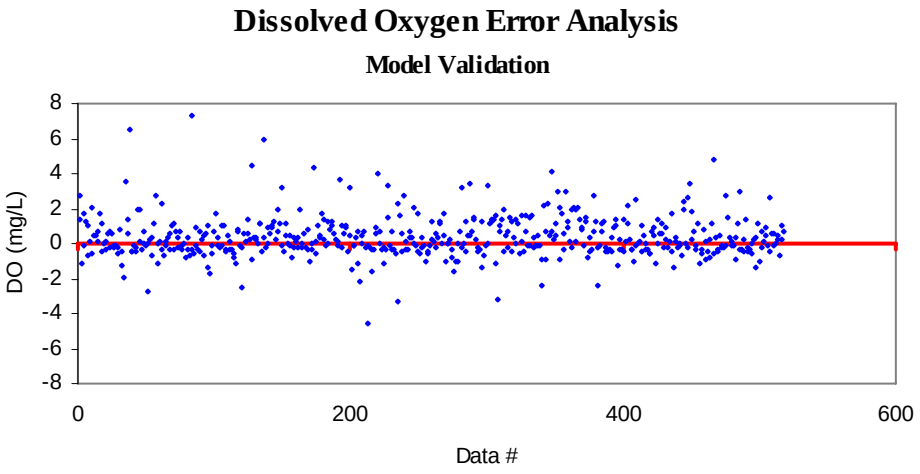


Figure 5-62. Dissolved Oxygen ANN Validation Model Error Analysis

The hourly receiving water DO model for site ESFSF013 discussed above was analyzed for sensitivity of different input parameters. Due to the strong correlation between temperature and DO, temperature has the greatest impact of all the input parameters used in the model.

5.3.2.3.4.2 ANN-based Daily-DO Inductive Model

In the daily DO inductive model, the inputs to the model consists of daily average stream flow, daily average temperature, daily average total nitrogen load, and daily average total phosphorus load. The output consists of the target daily average DO concentration in the receiving water at the point of interest in the watershed. The inductive model is used to predict DO at site ESFSF006, which is located downstream of the confluence of South and Middle forks of Beargrass Creek watershed (Figure 5-57). The stream flow data is obtained from the USGS gage stations in the watersheds as shown in Figure 5-57. Such a receiving water DO inductive model can be used to determine total nutrient load reduction strategies needed to bring the DO at site ESFSF006 within the regulatory limits.

Similar to the hourly DO model, the popular multi layer feed-forward back propagation neural networks were used in developing the daily DO inductive model. The model structure included one input layer, one hidden layer, and a corresponding output layer. The input layer consists of four input nodes representing daily stream flow (Q), temperature (T), total nitrogen load (TN), and total phosphorus (TP). The output layer consists of one node representing the target DO concentration (DO). The number of hidden nodes (H) in the hidden layer was varied in the model development, starting with five nodes and going up to a maximum of twelve nodes. A general schematic of the ANN structure used in developing the DO inductive model is given below in Figure 5-63.

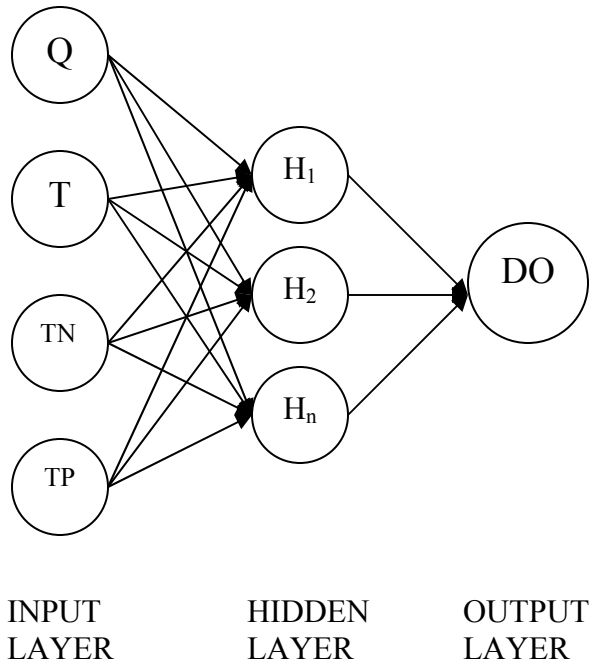


Figure 5-63. Neural Network Structure for Daily Inductive DO Model

The ANN network architecture was varied by using different number of hidden nodes in the hidden layer and varying the learning rate and momentum rate parameters. In the majority of evaluations, the most optimal results were obtained by using five hidden nodes in the hidden layer.

Data from October 1, 2003 through September 30, 2004 was used in the ANN-based daily average DO inductive model resulting in a total of 342 data points after disregarding the days for which no data was recorded. Figure 5-64 shows the average daily flow and average daily dissolved oxygen data for this period. Figure 5-65 shows the average daily temperature and average daily DO data for this period.

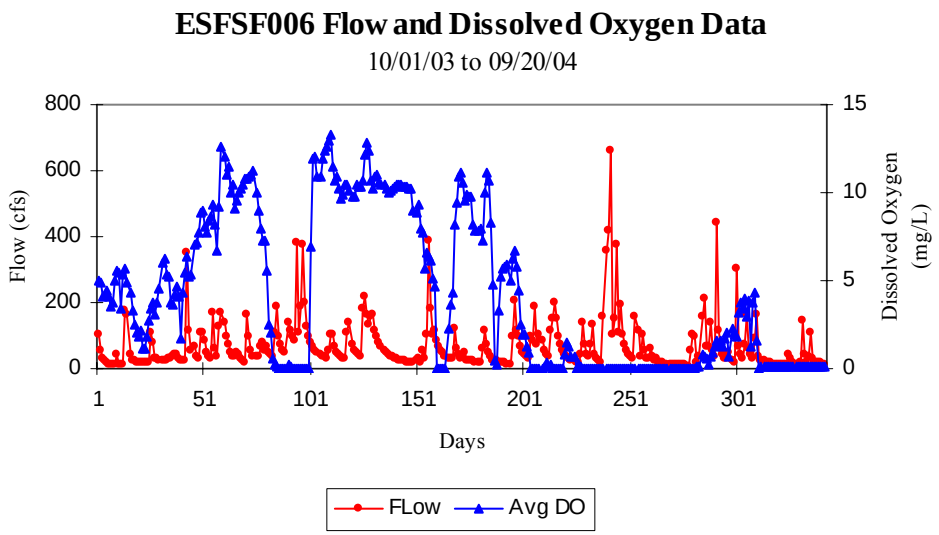


Figure 5-64. Flow and DO data for Site ESFSF006 (South Fork)

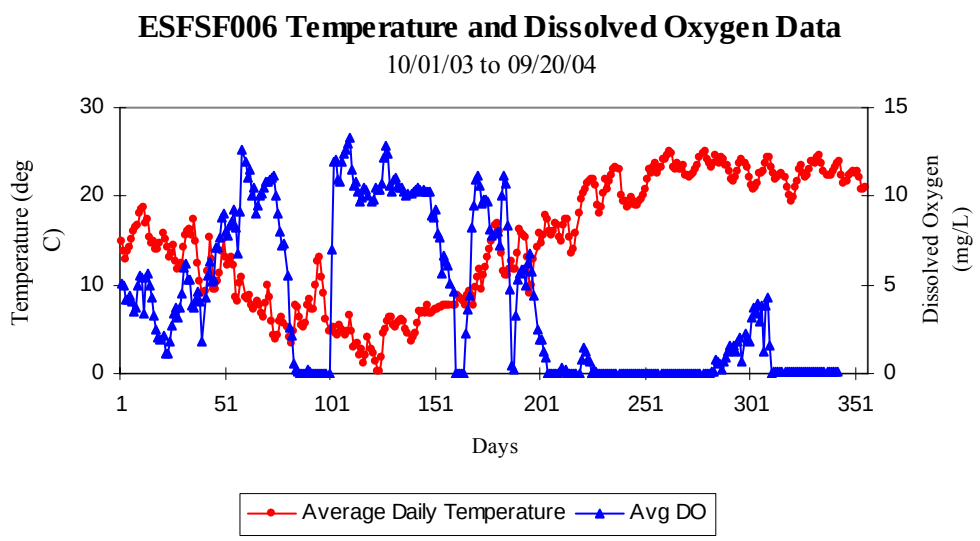


Figure 5-65. Temperature and DO data for Site ESFSF006 (South Fork)

The significant feature to note in the Flow-DO plot above (Figure 5-64) is the DO crashes that occur after a significant storm event. The crash seems to occur not immediately after

the storm event but is lagged by one or more days. This would imply that the storm event brings a load of oxygen consuming material and it takes a day or more for that material to be consumed by the oxygen demanding organisms in the column of water.

The ANN model structure as shown in Figure 5-63 with four inputs was not able to capture the observed DO dynamics within a reasonable confidence limit and resulted in a model that performed poorly (coefficient of determination ranging from 0.3 to 0.5). This can be attributed to the fact that since most of the DO crashes occur with a lag of one or more days after the storm event, a model with just daily values of flow and nutrient loads would not be able to model the DO crashes as observed in Figure 5-64 (flow-DO plot) above. Keeping this in mind, two more ANN model structures were analyzed and these included:

1. An ANN model in which the input data includes average daily nutrient loads (total nitrogen and total phosphorus) and average daily temperature values for up to 14 days (lagged from the current day).
2. An ANN model in which the input data includes average daily flow and average daily temperature values for up to 14 days (lagged from the current day).

Using current and previous days of data in the model would help in capturing the effect of flow and nutrient loads on the observed DO, in particular the crashes observed in the data. The inclusion of the 14-day lagged input parameters in the ANN model resulted in significant improvement in the prediction performance of the DO model. The model was able to capture with reasonable confidence the DO crashes as seen in the flow-DO plot. The results of these two types of models are provided as follows. It should be noted that flow and nutrient inputs are in some way analogous due to the high correlation that exists between the two parameters. This is evident from the nutrient models developed and discussed in the preceding section. However, the ANN-based average daily DO models using flow or nutrients as model inputs may vary slightly due to the lagged effect of the two inputs on the observed DO.

ANN-based DO Inductive Model with Nutrients and Temperature as Model Inputs (current and up to 14-day lag)

The ANN model structure is given in the Figure 5-66 below in which TN represents the average daily total nitrogen load, TP is the average daily total phosphorus load, and T is the average daily temperature.

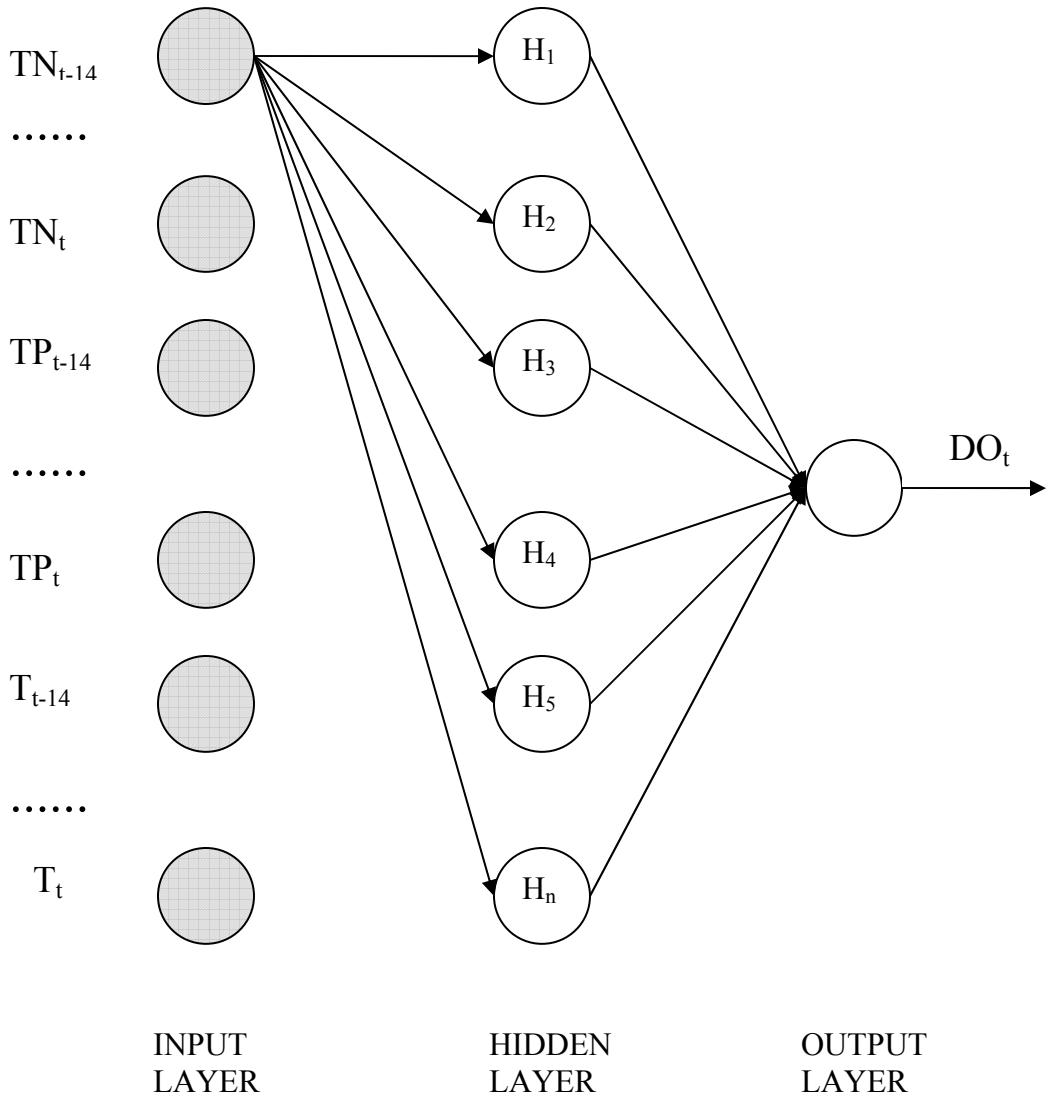


Figure 5-66. ANN DO Model Structure with Nutrient and Temperature Inputs

The ANN model consists of 45 inputs (15 total nitrogen load values, 15 total phosphorus load values, and 15 average daily temperature values). The number of hidden nodes in the hidden layer were varied from 10 to 30 and 15 hidden nodes in most cases gave the best model results. Figure 5-67 and 5-68 below shows the actual versus predicted DO from the ANN-based inductive model in training as well as validation. Figure 5-69 shows the actual and predicted time series of DO predicted by the ANN-based inductive model.

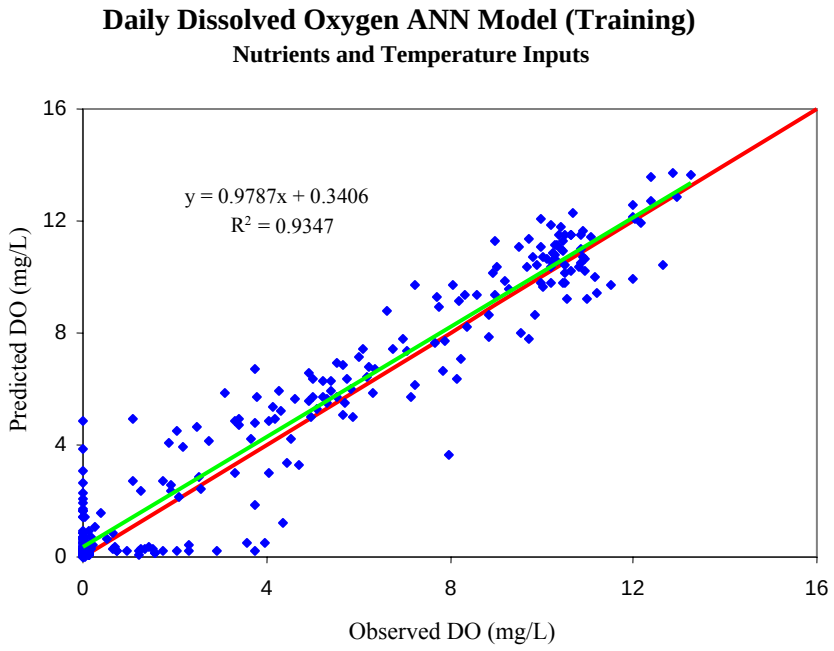


Figure 5-67. Performance of the Daily DO ANN Model in Training

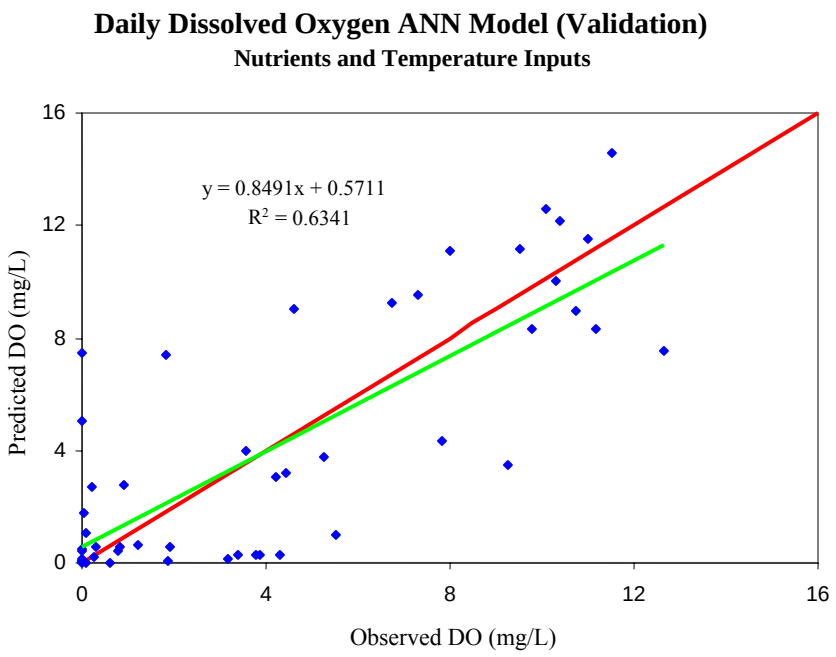


Figure 5-68. Performance of the Daily DO ANN Model in Validation

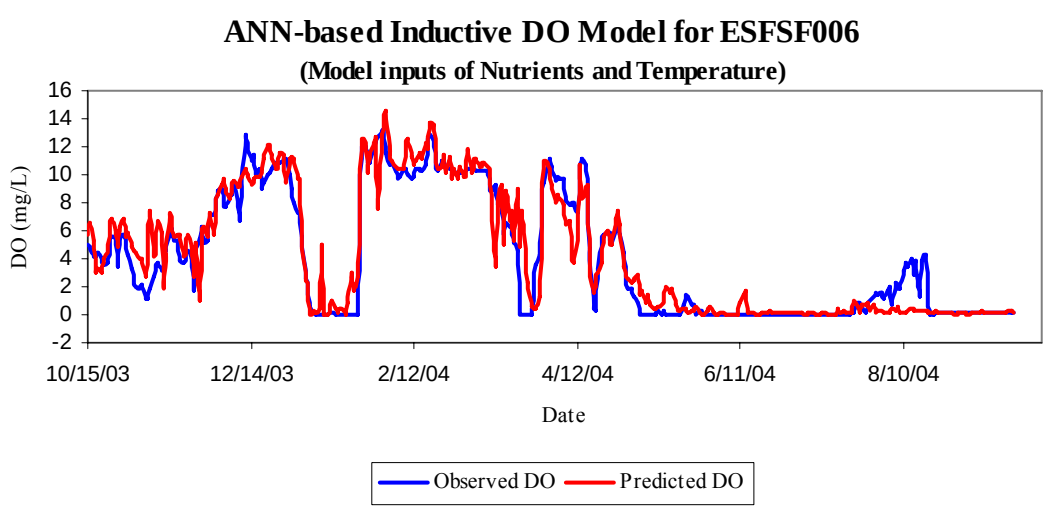


Figure 5-69. Time series of Daily DO from the ANN Model

Table 5-22 below gives the measures of performance for the DO model in training and validation.

Table 5-22. Measure of Performance of the Dissolved Oxygen ANN Model (Nutrients and Temperature as Model Inputs)

Model Type	Coefficient of Determination ($R^{2)}$	Mean Square Error (MSE)	Average Absolute Error	Maximum Absolute Error
Training	0.93	1.34	0.79	4.88
Validation	0.63	7.49	2.05	7.46

An error analysis was carried out for the ANN model in training and validation to demonstrate that the error is randomly distributed and there is no significant trend followed. The error graphs for the ANN model in both training and validation are shown in Figures 5-70 and 5-71 below.

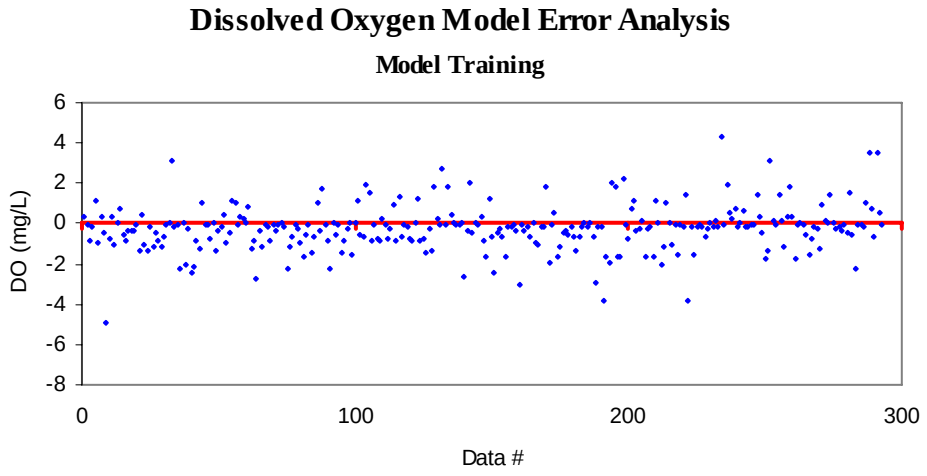


Figure 5-70. Error Analysis of the ANN Model in Training

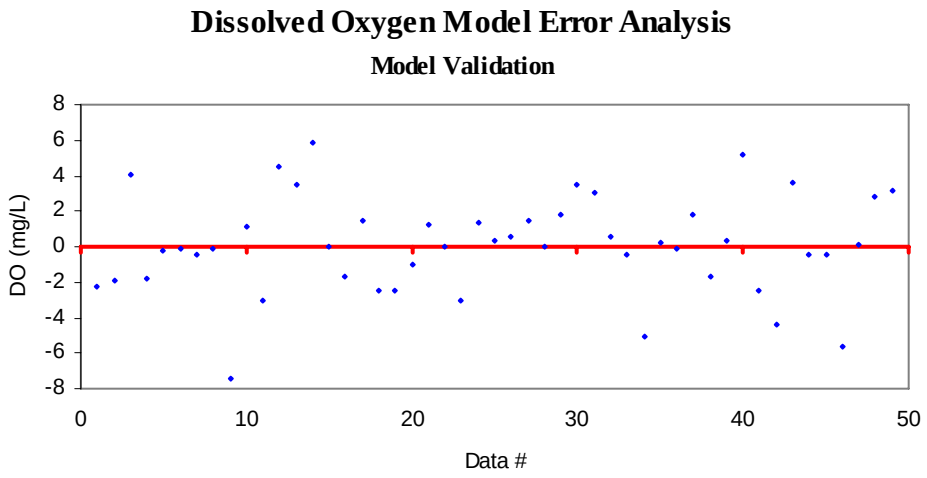


Figure 5-71. Error Analysis of the ANN Model in Validation

<u>ANN-based DO Inductive Model with Stream Flow and Temperature as Model Inputs (current and up to 14-day lag)</u>

The ANN model structure is given in the Figure 5-72 below in which Q represents the average daily stream flow, and T is the average daily temperature. The ANN model consists of 30 inputs (15 daily average flow values, and 15 average daily temperature values). The number of hidden nodes in the hidden layer were varied from 10 to 30 and 15 hidden nodes in most cases gave the best model results. Figure 5-73 and 5-74 below shows the actual versus predicted DO from the ANN model in training as well as validation. Figure 5-75 shows the actual and predicted time series of DO predicted by the ANN model.

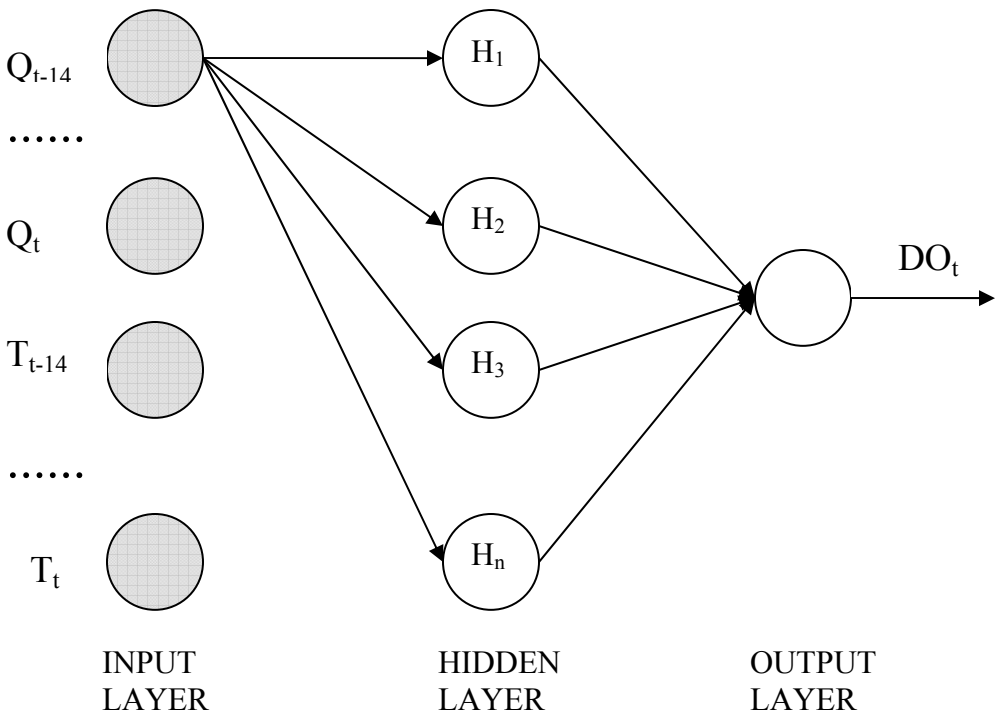


Figure 5-72. ANN DO Model Structure with Flows and Temperature Inputs

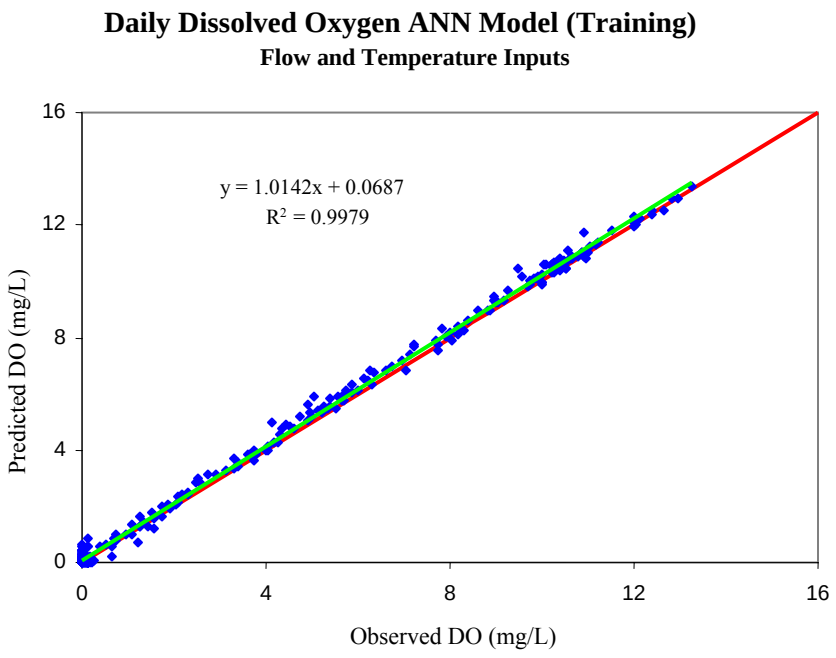


Figure 5-73. Performance of the Daily Dissolved Oxygen ANN Model in Training

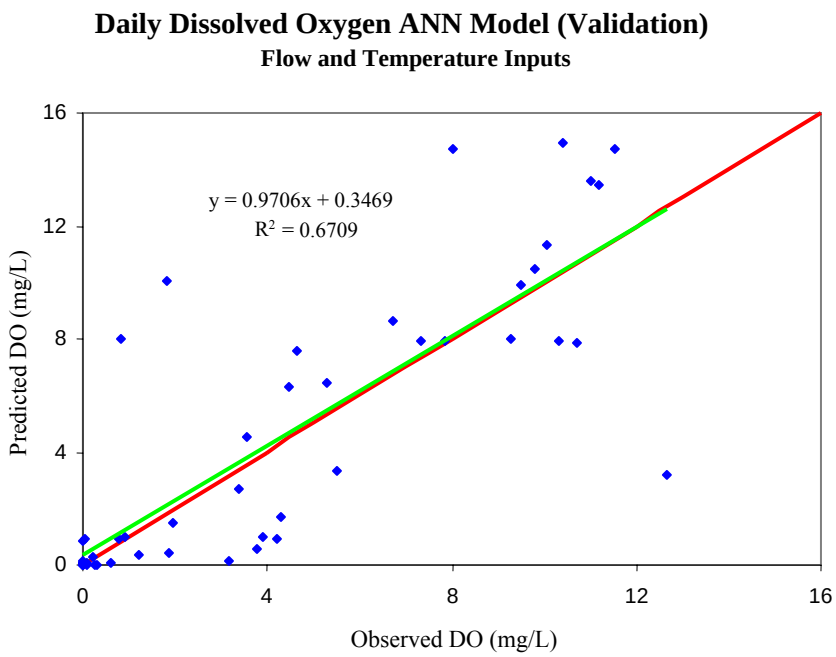


Figure 5-74. Performance of the Daily Dissolved Oxygen ANN Model in Validation

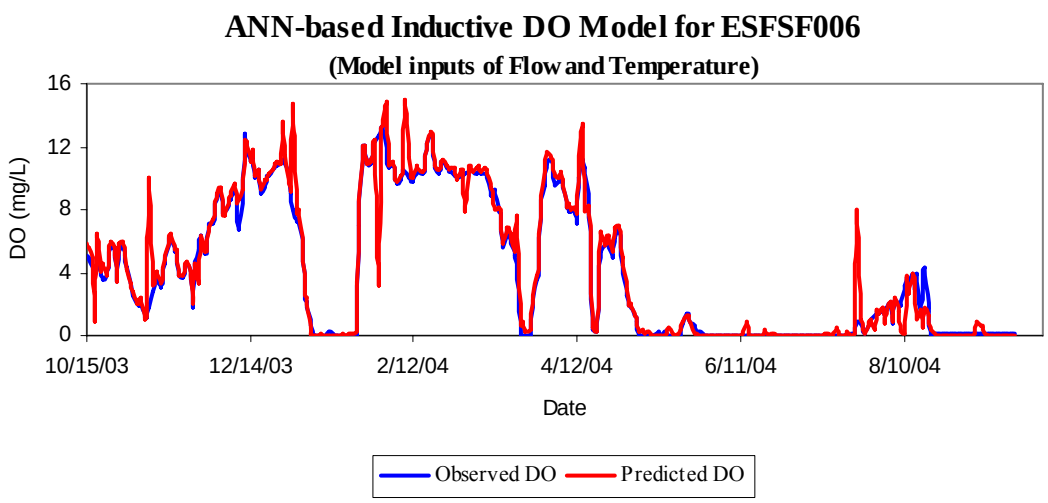


Figure 5-75. Time series of Daily Dissolved Oxygen from the ANN Model

Table 5-23 below gives the measures of performance for the DO model in training and validation.

Table 5-23. Measure of Performance of the Dissolved Oxygen ANN Model (Flow and Temperature as Model Inputs)

Model Type	Coefficient of Determination ($R^{2)}$	Mean Square Error (MSE)	Average Absolute Error	Maximum Absolute Error
Training	0.99	0.06	0.18	0.93
Validation	0.67	7.95	1.77	9.49

An error analysis was carried out for the ANN model in training and validation to demonstrate that the error is randomly distributed and there is no significant trend followed. The error graphs for the ANN model in both training and validation are shown in Figures 5-76 and 5-77 below.

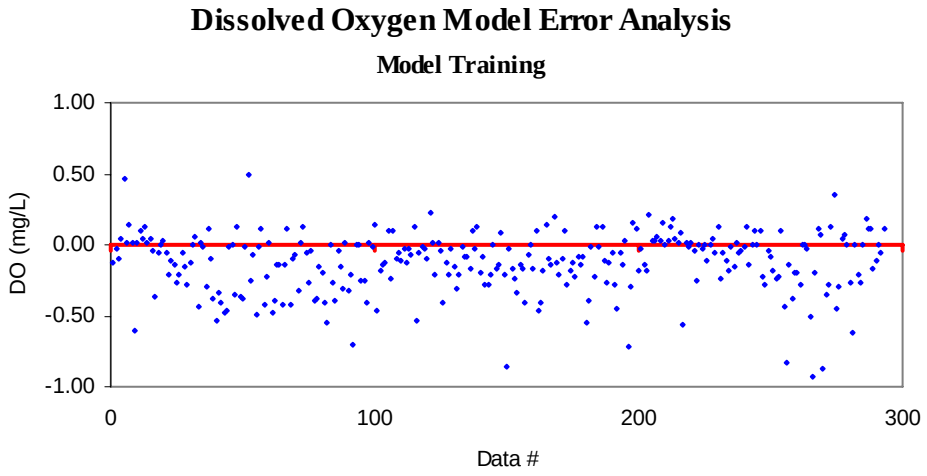


Figure 5-76. Error Analysis of the ANN Model in Training

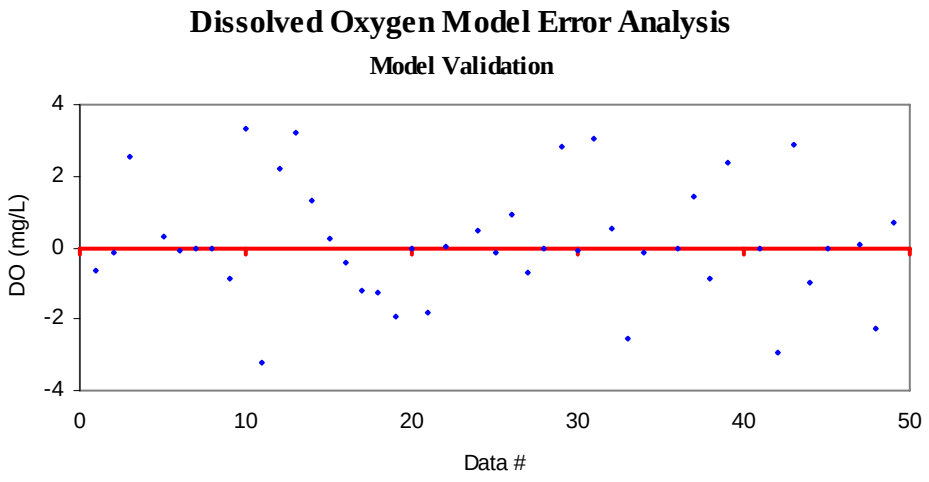


Figure 5-77. Error Analysis of the ANN Model in Validation

5.3.2.3.5 Summary of Results for DO Inductive Models

Three different types of inductive DO models based on ANNs were described in the previous sections. These include an hourly DO model with five inputs (Q, T, C, TN, and TP), an average daily DO model with 45 inputs (15 values of T, 15 values of TN, and 15 values of TP), and an average daily DO model with 30 inputs (15 values of T and 15 values of Q). The results show that ANN is capable of modeling the DO response in the stream based on the model inputs identified. The measure of performance of the ANN models included the coefficient of determination (R^2), mean square error (MSE), average absolute error, and maximum absolute error. All three models give varying degree of accuracy in predicting the DO. As a prediction tool, all three models perform reasonably well to capture the DO dynamics. The next test was to use these models as a management tool to establish load reductions necessary to improve the DO to above the regulatory limits. Using a trained ANN model, the inputs were modified to reflect a reduction in the nutrient loads and the modified inputs were evaluated using the DO inductive models. The models failed to respond in a favorable manner to the reductions applied in the stream flows or nutrient loads. Even though there was slight improvement in the DO with reduced nutrients, a more definite cause-and-effect relationship could not

be established as would be needed for the model for it to be used as a management tool for evaluating different reduction strategies. This is a significant finding and it points out an important fact that even though an inductive model may fit well to the given data and be an accurate prediction tool, it may lack the ability to be used as a management tool. For an inductive model to be effective for use as a management tool, it should be able to provide a reasonably accurate cause-and-effect relationship between inputs and outputs. Also, the cause-and-effect relationship provided by the model needs to be practical and reflective of the real world processes. The inability of the ANN models to provide a more realistic cause-and-effect relationship can be attributed to many reasons such as:

- The raw data used in the model development may be erroneous.
- The fact that ANN is a black-box model and does not understand the underlying processes and relationships of the inputs and outputs of the model.
- One or more model inputs may have a significant impact on the model output rendering other model inputs (particularly the ones for which load reductions are sought) rather insensitive to the model output (DO). For instance, temperature is strongly related to DO and may be driving the response of DO causing other model inputs such as flow and nutrients less effective in impacting the output.
- The model inputs for which reductions are sought may in reality have no significant impact on the model output. For instance, the stream flow and/or nutrients may not be causing the DO to crash as seen in the time series of observed data (Figure 5-64).

Due to reasons such as those outlined above, it can be stated that the ANN-based inductive DO models may serve as effective prediction tools as a function of inputs such as flow, temperature, and nutrients. However, these models will have little utility when used in a management framework to obtain optimal load reductions for water quality management. For use in a management framework, it is important to establish a cause-and-effect relationship between model inputs and outputs.

5.4 Simple Deductive Simulation Models

This type of macro-level models represents a simplified form of a complex process-based model to represent a response function being modeled. A complex water quality model for watershed management such as HSPF (Hydrologic Simulation Program Fortran) is usually developed to represent a variety of water quality processes (parameters of interest) occurring in the watershed such fecal coliform, dissolved oxygen, nutrients, biochemical oxygen demand, etc. Such a model when calibrated and verified, represent a cause-and-effect relationship between sources of pollution and in-stream concentration of pollutants under study. Such a complex model or suite of models can be broken down into simpler pieces with each piece representing the response of an individual process or a water quality parameter. Each individual process or parameter can then be modeled using a simplified mathematical representation to provide a simple deductive simulation model that can be used on a macro-level for water quality management. Examples of simple deductive models in hydrology and water quality modeling are given as follows:

1. The Kinematic Storage Method is a simplified version of the fully dynamic Saint Venant equations (conservation of mass and momentum equations).
2. The Green and Ampt equation for modeling infiltration is a simplification of the Richard's equation for infiltration that involves partial differential equations.
3. The Streeter-Phelps model for modeling dissolved oxygen deficit is a simplification of the advection-diffusion contaminant transport equation.

5.4.1 Example Application

To demonstrate the concept of simple deductive model for water quality modeling and subsequent use as a macro-level model in a water quality management framework, a simplified dissolved oxygen (DO) simulation model is developed for simulating DO in each of the three forks of Beargrass Creek watershed.

5.4.1.1 Simplified Deductive Dissolved Oxygen Model

The explicit inductive DO models described in the previous section reveals that while they can serve as good prediction models that fits well to a given set of input data, they have significant shortcomings when used in a management framework. The simple deductive DO model based on the classic Streeter-Phelps equation (Streeter and Phelps, 1925) is a motivation of the shortcomings resulting from the use of inductive DO models (as described in the previous section). An effort is made to construct a simplified DO model that can establish a reasonable cause-and-effect relationship between model inputs and model output (DO) and can be effectively used for determining load reductions. In this approach, it is hypothesized that the DO crashes observed in the data collected for the Beargrass Creek watershed (Figures 5-64 and 5-65) are largely due to the BOD loads contributed by different sources of pollution in the watershed. This hypothesis is justified by the following factors:

- The explicit inductive DO models based on stream flow, nutrients, and temperature were rather insensitive to the nutrient loads and stream flow used as model inputs.
- BOD loads caused mainly by CSO/SSO events are responsible for the chronic DO crashes, while the more acute and diurnal fluctuation of DO over a 24-hour period are related to nutrients and algae presence.
- The watershed does not seem to be nutrient limited and any reduction in nutrients may not significantly affect the DO, particularly in the case of the chronic crashes following a severe storm event (personal communication with Lynn Jarrett, 2005).

The Streeter-Phelps (Streeter and Phelps, 1925) model relates the DO deficit in a water body to the ultimate BOD concentration and can be effectively used to evaluate the impact of BOD load reduction on DO in a water body. Before the model development is described, it is important to understand the DO-BOD cycle and important processes occurring in such an interaction in a stream ecosystem.

5.4.1.1.1 DO-BOD Cycle in Stream Water

In a stream ecosystem there are many inter-connected processes occurring simultaneously that affect the DO levels in the water column. Figure 5-78 shows some of the most important processes occurring in a stream system that are usually considered in modeling DO. Oxygen in such an environment is produced by photosynthesis of algae and plants and is consumed by respiration of plants, animals and bacteria, BOD degradation process, sediment oxygen demand (SOD), and oxidation. It is re-aerated by the exchange of oxygen from the atmosphere.

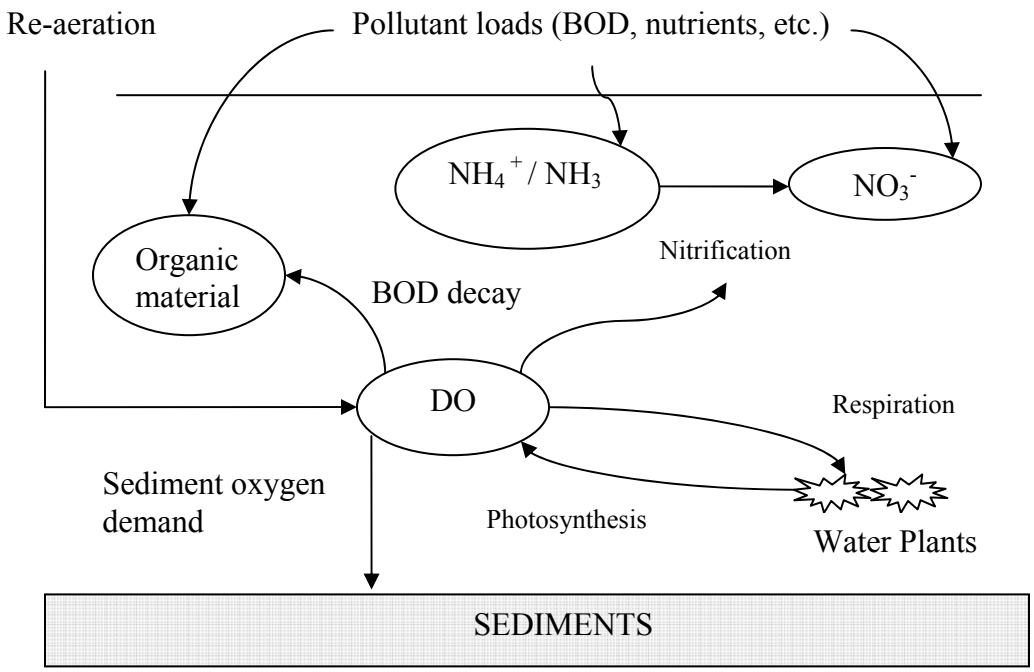


Figure 5-78. Processes related to modeling of DO (Radwan et al. 2003)

Similarly, Figure 5-79 gives an overview of the most important processes related to BOD modeling in a stream system. Degradation of the organic matter expressed as BOD results in the equivalent consumption of oxygen. Degradation of BOD is also a source of nutrients (NH_4-N) that are oxidized by oxygen and thus causing additional consumption of oxygen (Radwan et al. 2003).

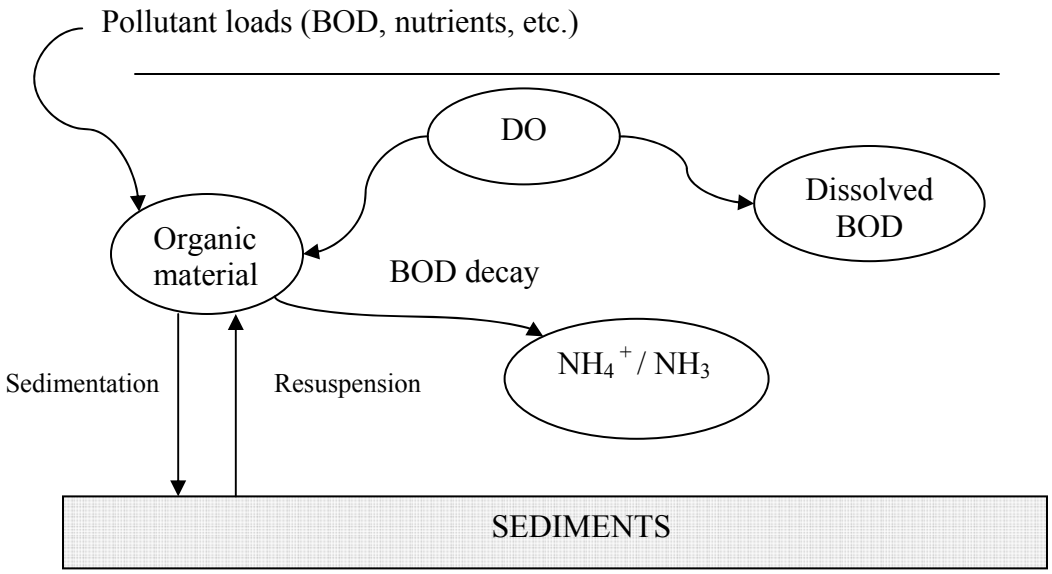


Figure 5-79. Processes related to modeling of BOD (Radwan et al. 2003)

5.4.1.1.2 Streeter-Phelps Dissolved Oxygen Model

A simple, conceptual, and macro-level steady state dissolved oxygen model was developed for each of the three forks of Beargrass Creek watershed using the classic Streeter-Phelps equations. The data set used in this model is the same that was used in the ANN-based Inductive DO models with a daily time step as described in the previous section and consists of the continuous DO and stream flow data for the period October 1, 2004 to September 30, 2004. Figure 5-80 shows the DO sampling sites as well as the five USGS stations at which rainfall data is collected.

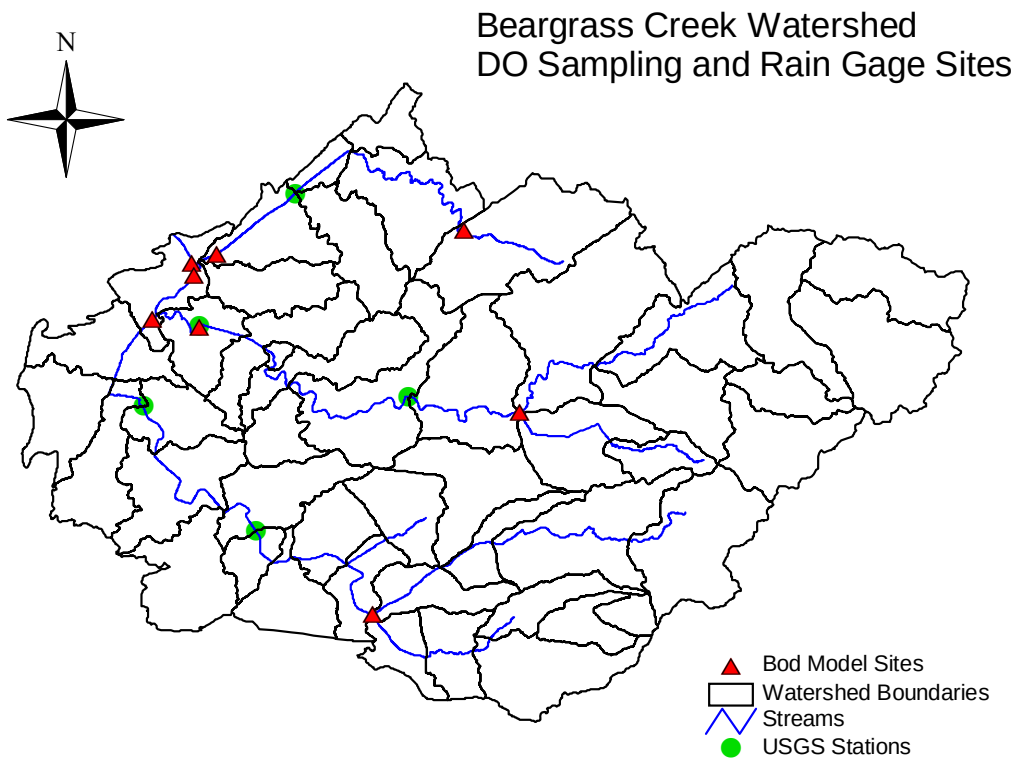


Figure 5-80. Dissolved Oxygen Sampling and Rain Gage Sites

Many computer programs and equations are used to simulate water quality in streams, rivers, and lakes. To model the DO deficit occurring in a stream, the most prevalent of such equations is the Streeter-Phelps equation (Streeter and Phelps, 1925). Being a simplified representation of the actual DO dynamics, a model based on the Streeter-Phelps equation has certain limitations due to the assumptions of the model. The assumptions of the simplified deductive DO model developed in this study based on the Streeter-Phelps equation are described as follows:

- Stream is an ideal plug flow reactor.
- Steady-state flow and BOD and DO reaction conditions.
- One dimensional stream flow is assumed.

- Effects of diffusion or dispersion are neglected.
- The only reactions of interest are BOD exertion and transfer of oxygen from air to water across air-water interface.
- Only carbonaceous BOD is exerted in the model.
- Both reoxygenation and deoxygenation are first order.

The dissolved oxygen in each of the streams, DO, depends on the oxygen deficit D and the saturation dissolved oxygen DO_{sat} as given by Equation (5-18). The oxygen deficit is a function of the initial deficit D_o, ultimate BOD concentration L_o, BOD decay rate K_d, and re-aeration from the atmosphere K_a, and is given by Equation 5-19 (Streeter-Phelps DO Model). Equation (5-20) is obtained by solving Equation (5-19) for the ultimate BOD concentration L_o and assuming that the initial deficit D_o is equal to zero. Figure 5-81 gives a sketch of the DO dynamics along the length of each of the streams. For simplification, the entire stream is considered one reach in the analysis starting at an upstream location where the DO is observed to be close to saturation and ending at the most downstream end of the stream.

$$DO = DO_{sat} - D \tag{5-18}$$

$$D = D_o\, e^{\left(\frac{-Ka}{U}\right)X} + \frac{K_d\, L_o}{K_a - K_d}\left(e^{\left(\frac{-Kd}{U}\right)X} - e^{\left(\frac{-Ka}{U}\right)X}\right) \tag{5-19}$$

$$L_o = \frac{(K_a - K_d)D}{\left(e^{\left(\frac{-Kd}{U}\right)X} - e^{\left(\frac{-Ka}{U}\right)X}\right)} \tag{5-20}$$

Where Do = initial deficit

L_o = ultimate BOD concentration (mg/L)

K_a = re-aeration rate (day)-1

K_d	=	decay rate (day)-1 for carbonaceous BOD
U	=	average velocity in the stream (feet per day)
X	=	length of the stream (feet)

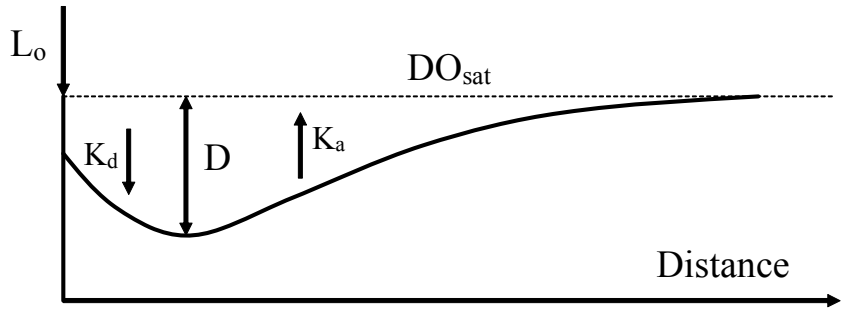


Figure 5-81. Dissolved oxygen deficit in the stream

A schematic of the stream segments in each of the three forks is given in Figure 5-82 below. The term D_o in Equation (5-19) is assumed zero since the model assumes saturation conditions at the upstream end of each of the three forks. This assumption is backed by the fact that observed DO data at the upstream end does not show any impairment and is close to the saturation DO value for most days of the model period (October 1, 2004 to September 30, 2004). A daily time step was used in the steady state dissolved oxygen model.

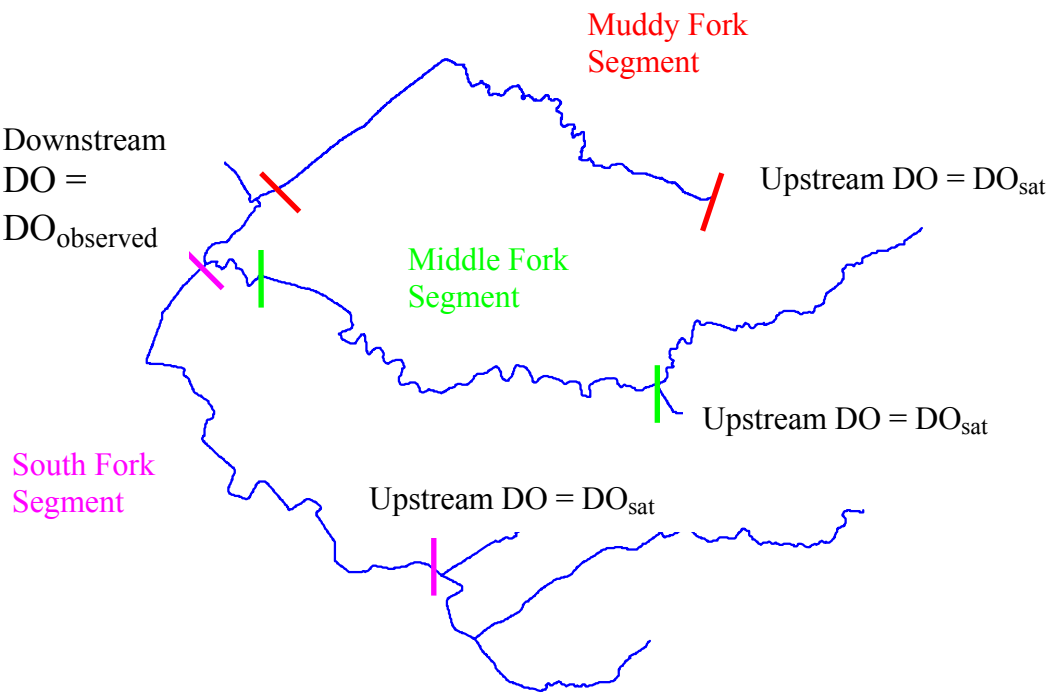


Figure 5-82. Schematic of the DO Model for three Forks in Beargrass Creek Watershed

Based on the actual average daily deficit observed between the most upstream and downstream stations of the stream, Equation (5-20) is used to back-calculate the ultimate BOD concentration (L_o) that is causing the average daily DO deficit observed. Initial deficit is assumed to be zero as the DO in the most upstream end of the each of the stream is fairly close to the saturation DO. The rate of decay (K_d) is assumed to be 0.25 (suggested range of 0.15 to 0.35 in most text books). The re-aeration rate (K_a) is computed based on the average velocity and depth in the stream by using Equation 5-21 (O'Connor and Dobbins, 1958), Equation 5-22 (Churchill et al. 1962), or Equation 5-23 (Owens, et al. 1964). The depth and velocity terms used in Equations 5-21 through 5-23 were computed by using relationships derived from actual rating curves developed for all of the USGS gauging stations of the watershed.

$$K_a = 12.9\left(\frac{Velocity^{0.5}}{Depth^{1.5}}\right) \quad (5\text{-}21)$$

$$K_a = 11.6\left(\frac{Velocity}{Depth^{1.67}}\right) \quad (5\text{-}22)$$

$$K_a = 21.6\left(\frac{Velocity^{0.67}}{Depth^{1.85}}\right) \quad (5\text{-}23)$$

The total average daily flow is obtained for each of the three forks by utilizing the data collected at five USGS gauging stations in the watershed. Average daily flow is segregated into three components corresponding to the three sources namely (as shown in schematically in Figure 5-83):

1. Point source flow from CSO discharges
2. Non-point source flow from urban runoff, and
3. Base flow in the stream.

The contribution of CSO flows for a particular stream reach is approximated by using USGS gauging stations upstream and downstream of the CSO areas as follows. First, the total contributing drainage area between the two USGA stations was determined and separated into a CSO drainage area and a non-CSO drainage area using the GIS coverage for the watershed. This will establish the percentage of CSO drainage area for a particular stream reach between the two USGS gauging stations. Second, the difference of stream flow is computed between the two USGS gauging stations on a particular stream reach. Lastly, the percentage of CSO areas computed in the first step is applied to the difference flow computed in the second step to get an approximation of the CSO component of the stream flow for a particular stream reach. The remaining flow is assumed to be contributed by storm water runoff due to the non-CSO drainage area in the stream reach. In addition, a constant base flow is assumed based on the actual total flow hydrograph obtained at the USGS sites.

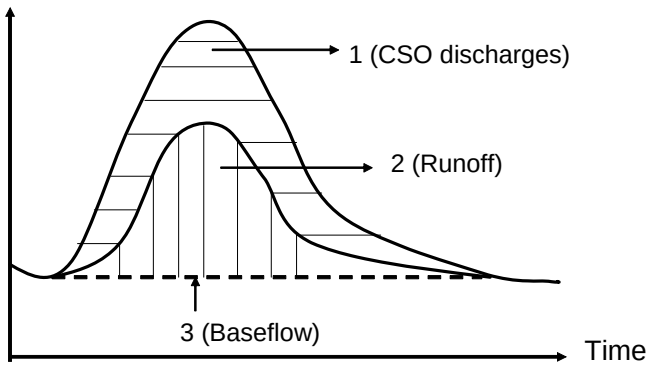


Figure 5-83. Segregation of daily average flows for each fork of Beargrass Creek

The ultimate BOD concentration (L_o) computed using Equation (5-20) represents a total effective BOD concentration (load) that is causing the DO deficit at the downstream end of the stream segment. Figure 5-84 below shows a schematic of a typical stream segment in which the effective load applied at the upstream end of the segment is causing the DO deficit observed at the downstream end. Figures 5-85 through 5-87 shows the effective total BOD concentration (L_o) time series computed for each of the three forks in the Beargrass Creek watershed for the period October 1, 2003 through September 30, 2004.

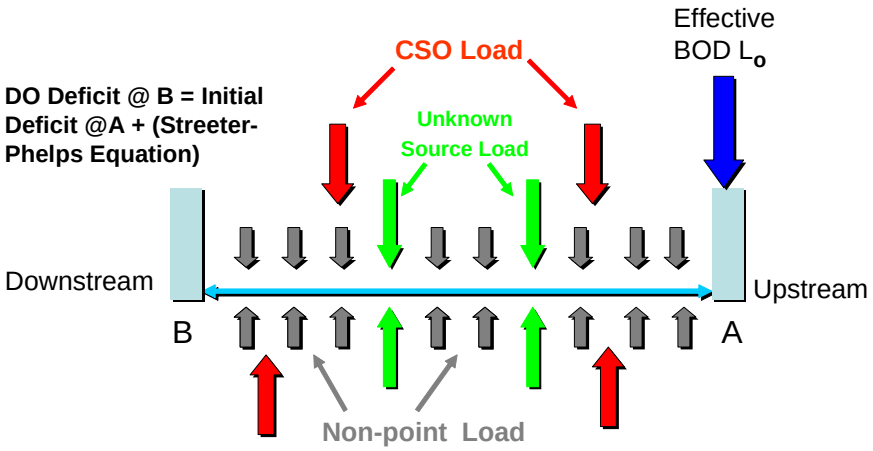


Figure 5-84. Schematic of BOD Load Application in the Deductive DO Model

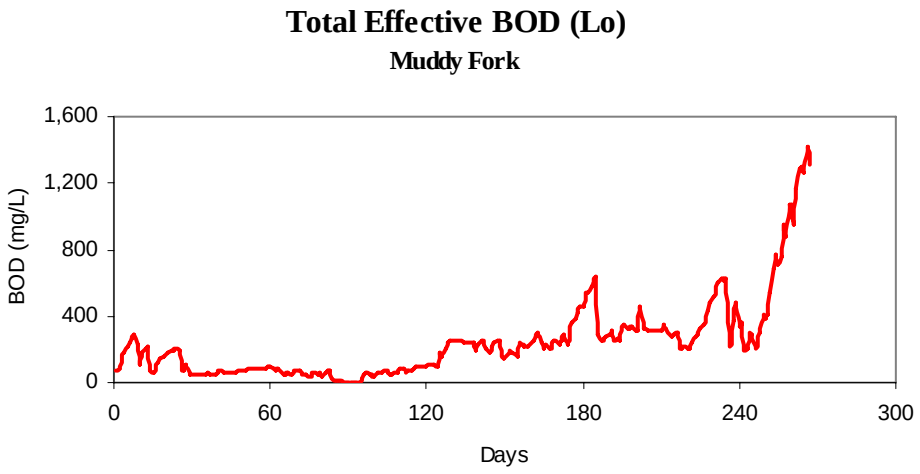


Figure 5-85. BOD Time Series computed for Muddy Fork Watershed

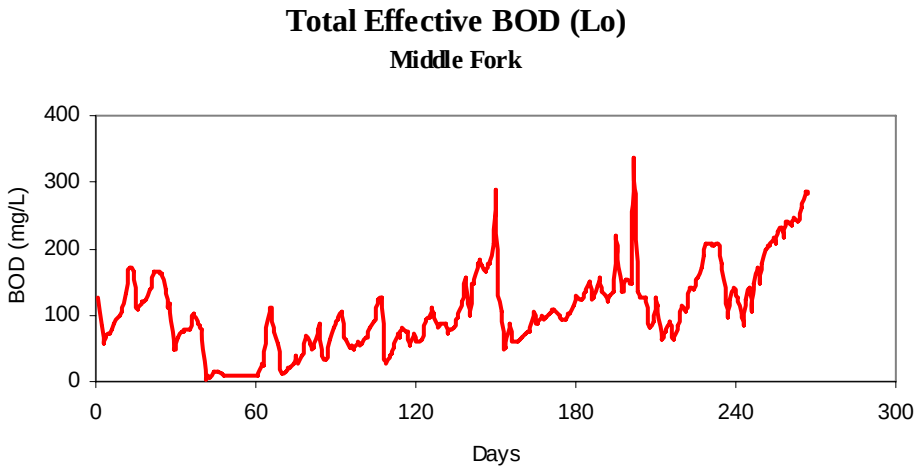


Figure 5-86. BOD Time Series computed for Middle Fork Watershed

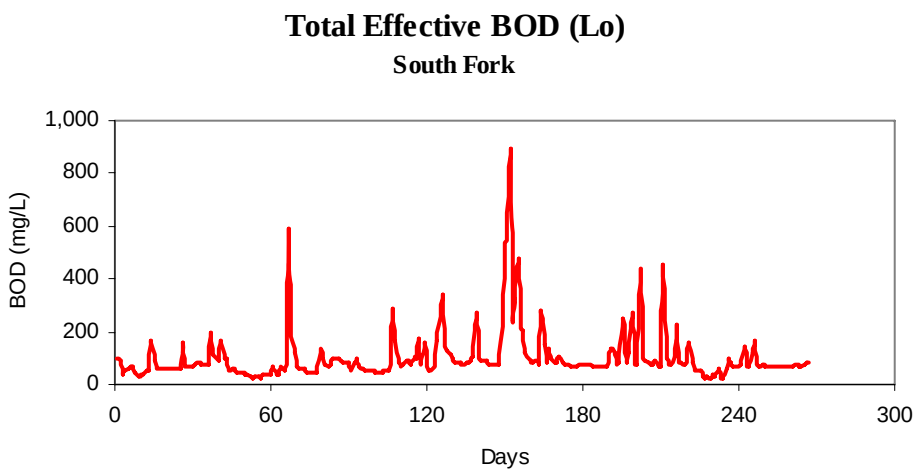


Figure 5-87. BOD Time Series computed for South Fork Watershed

Once the effective daily ultimate BOD concentration (L_o) is computed, a mass balance of flow and concentration for each of the contributing sources is performed to quantify the BOD concentration from each source. Three types of sources are identified to be contributing BOD loads into the stream segments including:

1. Point source contribution of BOD loads from CSOs events during storm event.
2. Non-point source contribution of BOD loads from storm water runoff.
3. An unknown or undetermined source of BOD contribution that is associated with the base flow in the streams. Such an unknown source may include other suspected sources of BOD contribution such as sediment oxygen demand (SOD) or ex-filtration from leaking sewers (that run close to the stream segments in the model) onto the stream banks.

The total BOD concentration (calculated from Equation 5-20 above) can be represented as a mass balance of the flow and concentration from the three sources of flow and BOD concentration identified above and is given by Equation 5-24 below.

$$L_o\ (Total\ BOD) = \left(\frac{Q_{PS} * L_{PS} + Q_{NPS} * L_{NPS} + Q_{BF} * L_{UKS}}{Q_{PS} + Q_{NPS} + Q_{BF}} \right) \tag{5-24}$$

Where	L_o	=	total ultimate BOD concentration in mg/L
	Q_{PS}	=	point source flow (CSO discharges) in ft3/sec
	Q_{NPS}	=	non-point source flow (urban runoff) in ft3/sec
	Q_{BF}	=	base flow in ft3/sec
	L_{PS}	=	BOD concentration of CSO discharges in mg/L
	L_{NPS}	=	BOD concentration of urban runoff in mg/L
	L_{UKS}	=	BOD concentration of the unknown source

BOD concentration values were assigned to the point and non-point source contributions based on a survey of literature values (Tetra Tech, 2005) and used in Equation 5-25 to obtain the BOD concentration for the unknown source. Literature values used for L_{PS} = 50 mg/L and L_{NPS} = 10 mg/L. These can obviously be changed if actual values are available either from sampling or as an output from a more detailed process-based model of the watershed.

$$L_{UKS} = \frac{\left(L_o * \left(Q_{PS} + Q_{NPS} + Q_{BF}\right) - \left(Q_{PS} * L_{PS}\right) - \left(Q_{NPS} * L_{NPS}\right)\right)}{Q_{BF}} \tag{5-25}$$

Once the unknown source BOD concentration is determined from Equation (5-25), the model can be used in the forward direction to compute DO at the downstream end of each of the three forks of the Beargrass Creek watershed. A mass balance of DO and flows is performed to compute the DO at the confluence of the forks. This is done at two locations in the model; first at the confluence of South and Middle forks, and second at the confluence of South and Muddy forks. The resulting DO time series for the three

forks of Beargrass Creek watershed and the two confluence locations are given in Figures 5-88 through 5-92. As expected, the DO time series obtained using the simplified deductive model matches the observed DO at the outlet of the three sub-watersheds and the downstream confluence locations of the Beargrass Creek watershed.

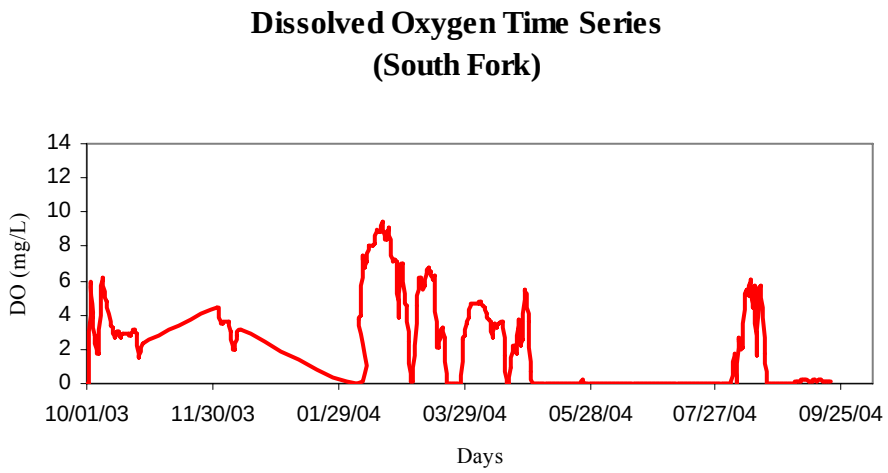


Figure 5-88. South Fork DO Time Series using Simplified Deductive Model

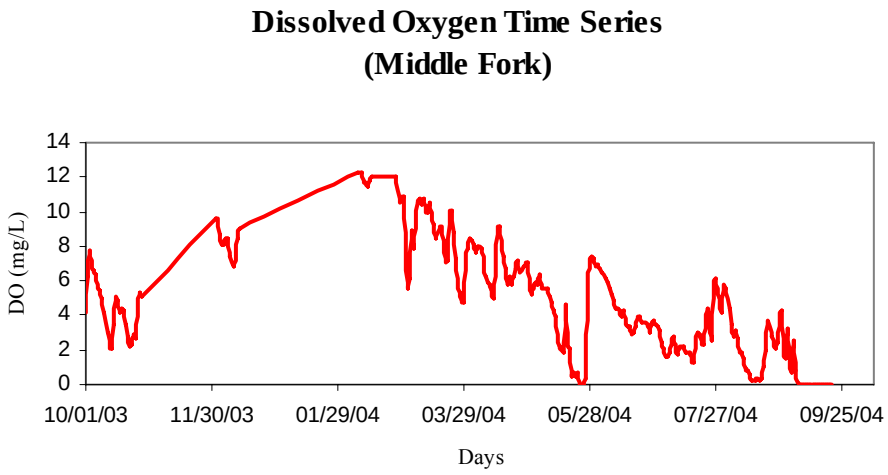


Figure 5-89. Middle Fork DO Time Series using Simplified Deductive Model

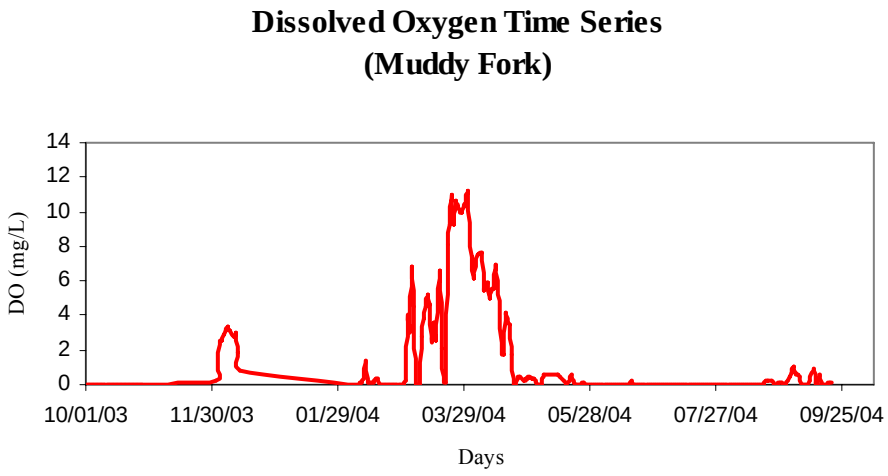


Figure 5-90. Muddy Fork DO Time Series using Simplified Deductive Model

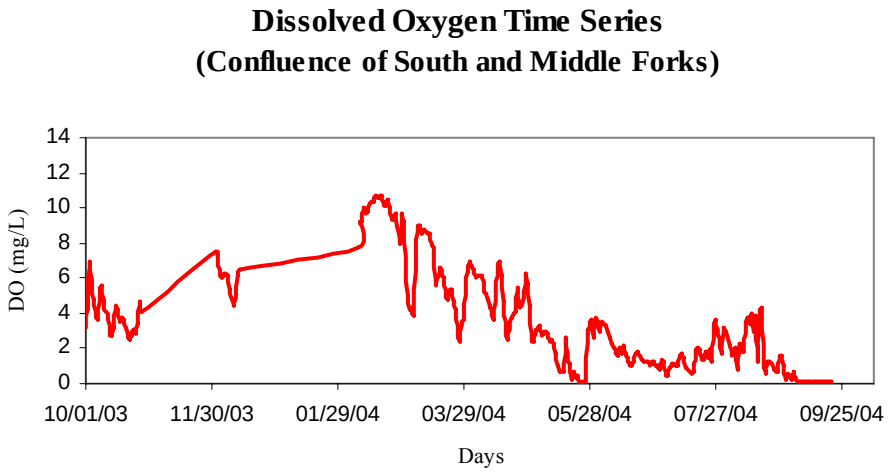


Figure 5-91. South-Middle DO Time Series using Simplified Deductive Model

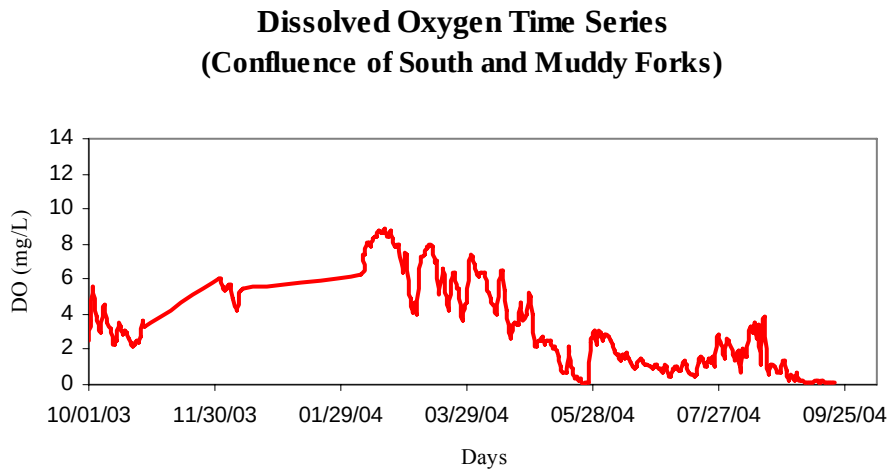


Figure 5-92. South-Muddy DO Time Series using Simplified Deductive Model

5.4.1.1.3 Summary and General Remarks

A simplified macro-level DO simulation model based on the Streeter-Phelps equation was developed using observed DO deficit data for the three forks of the Beargrass Creek watershed. This macro-level simple deductive approach results in a simple DO simulation model that is calibrated with observed data. The model is capable of establishing a cause-and-effect relationship between organic loads (BOD) and DO in the streams. Such a simplified DO-BOD load model can be very useful for use in an optimal management formulation to evaluate different water quality management strategies for BOD load reduction. For instance, by varying any or all of the six terms on the right side of Equation (5-23) which includes Q_{PS}, Q_{NPS}, Q_{BF}, $L_{PS,}$ L_{NPS}, and L_{UKS}, a new value of the total ultimate BOD load (L_o) can be computed for each of the three forks. The modified total BOD concentration (L_o) for each stream segment can then be used in the forward model using Equation (5-19) to compute the corresponding DO deficit. This will allow the evaluation of different flow reduction and BOD concentration reduction strategies for all three stream segments in a management framework resulting in the improvement of DO in the water bodies. Such a model will be more effective for evaluating management strategies because the Streeter-Phelps equation provides a very direct cause-and-effect

relationship between the effective total BOD concentration (L_o) and the corresponding DO deficit in the stream reach being analyzed.

CHAPTER 6
THE OPTIMAL WATERSHED MANAGEMENT MODEL

6.1 Introduction

Increased urbanization in watersheds as a result of growth in U.S urban corridors is causing an increase in water pollution problems and a deterioration of the water quality of water bodies. Integrated watershed management approach is increasingly being used to solve such problems. Such an approach can lead to identification of management strategies for water quality management. While acknowledging the problems of urbanization in watersheds and its associated impacts on water bodies, there is a need to further develop the science of integrated watershed management. Such a need requires scientists, engineers, and all stakeholders in a watershed framework to work towards developing effective water quality management strategies for urban watersheds. Such strategies can be developed by using principles of hydrology, water quality, computer-based modeling, and the various techniques of operations research (optimization) in an integrated watershed management framework. In principle, an effective management strategy for urban watersheds should be cost-effective, practical, and should satisfy all water quality objectives for the watershed. The strategy should be comprehensive in that it should address both point, non-point, and other undetermined sources of pollution that may exist in the impaired watershed. This has been the primary motivation of this research and an optimal management model for urban watersheds is presented here that can be effectively used to evaluate multiple management strategies resulting in optimal strategies (strategies that are cost effective and meet water quality objectives).

6.2 Previous Work

There are many applications of optimization techniques in general and evolutionary methods (such as genetic algorithms) in particular in the area of water resources engineering and management. These range from calibrating watershed or water quality simulation models to selecting optimal storm water management strategies to identifying

optimal load reduction strategies for water quality management. Broadly speaking, the use of optimization for water quality and/or watershed management falls into two categories namely 1) those studies in which optimization is used to enhance a simulation model (such as calibration and error correction), and 2) those studies in which optimization is used to achieve optimal management strategies (such as storm water quality and river water quality). In the current research, optimization is used in an integrated watershed management framework to achieve optimal water quality load reductions by coupling with a macro-level simulation model. In the past, there have been few applications of evolutionary algorithms for such integrative modeling for watershed management (Muleta, 2003). A brief description of some of the more recent contributions in the use of optimization models coupled with water quality simulation models for water quality and/or watershed management is given as follows.

- Muleta (2003) developed an integrative computational methodology for the management of non-point source pollution from watersheds. The method is based on an interface between evolutionary algorithms (EAs) and a comprehensive watershed simulation model known as Soil and Water Assessment Tool (SWAT). The decision support system developed is capable of identifying optimal land use patterns to satisfy environmental and economic related objectives. The study also uses a simple genetic algorithm to calibrate the SWAT model thus improving its ability to accurately predict stream flows and sediment yields. The resulting calibrated SWAT model is used with a simple GA for single objective optimization and with a Strength Pareto Evolutionary Algorithm for multi-objective optimization. Finally, the study also investigates the utility of an alternative inductive model based on Artificial Neural Networks (ANN) that is trained on the output of a calibrated SWAT model as a substitute for the computationally expensive SWAT model in the management framework.
- Vrugt et al. (2003) and Vrugt et al. (2003) developed efficient and effective optimization algorithms for estimating parameter uncertainty and calibration of hydrologic models. The work described in these studies uses a Markov Chain Monte Carlo (MCMC) sampler called the Shuffled Complex Evolution Metropolis

algorithm (SCEM-UA) for parameter estimation and a Multi-objective Shuffled Complex Evolution Metropolis algorithm (MOSCEM) for calibration of hydrologic models. Both the SCEM-UA and MOSCEM are derived using the Shuffled Complex Evolution approach of Duan (1993) and the unconstrained optimization method of Nelder and Mead (1965).

- Dorn (2004) developed a new evolutionary algorithm based technique for systematic generation of alternatives and multi-objective optimization to aid in watershed management. The new EA-based framework focused on storm water management issues such as use of best management practices (BMPs) to control runoff resulting from new developments. In particular, the modeling and management framework was applied to watersheds for obtaining cost-effective system of pipes and dry detention ponds to convey runoff generated by a design storm while meeting objectives of runoff control. The optimization model developed in the study works in conjunction with a storm water simulation model (called SWMM – Storm Water Management Model) developed by EPA.
- Mujumdar and Subbarao (2004) presented a fuzzy waste load allocation model for water quality management of a river system. The model uses a GA coupled with a steady state water quality simulation model called QUAL2E. A GA is used as an optimization tool to find optimal fraction removals of BOD load from various dischargers into the river system while maintaining required levels of dissolved oxygen in the system. A decoder-based method called homomorphous mapping (HM) is used to handle constraints using GA in this application. A similar model is presented by Burn (2001) in which GA is used to identify solutions to the waste load allocation problem. The constraints are handled through the use of penalty coefficient method. If a solution is identified that results in one or more violations, the cost of treatment corresponding to that solution is increased by an amount that is a function of the number of violations and the magnitude of the sum of violations (Burn, 2001).
- Goktas and Aksoy (2004) presented the application of GA for calibration and verification of a QUAL2E model. The GA is used to determine the re-aeration coefficient for the water quality simulation model called QUAL2E.

- Durga Rao and Satish Kumar (2004) presented a GIS-based decision support system for supporting watershed management practices related to soil erosion.
- Zechman (2005) developed a new method to improve the predictive capabilities of simulation models for use in watershed management. The work results in new evolutionary computation (EC) based methods to generate alternatives for numeric and symbolic search problems. This work is focused more on the simulation model component of the overall watershed management framework and finding new EC-based methods for enhancing alternative generation capabilities of search algorithms for use in error correction of simulation models.

6.3 Current Work

In the current research, optimization is used in an integrated watershed management framework to achieve screening-level optimal water quality load reductions. This is achieved by coupling macro-level water quality simulation models with efficient optimization models in a linked nonlinear constrained optimization framework. Given the complexity and nonlinear nature of water quality processes occurring in an urban watershed subject to multiple sources of pollution including point and non-point sources, evolutionary algorithms were selected as one of the method of optimization in this research. The fact that evolutionary methods work with a population of solutions, thus providing many alternative solutions favors its application to watershed management problems. Different feasible alternative solutions will provide multiple management scenarios for watershed managers leading to the ultimate selection of the most effective strategy that meets economic, environmental (water quality), and other specified goals. In particular, a genetic algorithm is applied in a coupled simulation-optimization approach to the problem of water quality management for urban watersheds. For comparison purposes, the performance of the GA algorithm is compared with a new Shuffled Box Complex method of constrained optimization, which is based on the original Box Complex method (Box, 1965). The Box Complex (Box, 1965) method is modified from its original version by initializing multiple complexes (as opposed to one complex) and randomly shuffling the vertices of the complexes after a specified number

of generations (iterations). Such an approach of multiple complexes and random shuffling is assumed analogous to the search mechanism in evolutionary methods making it more robust than the original Box Complex method.

6.4 Optimal Management Model Formulation

A disaggregated approach of optimal management formulation is used in the proposed management model. Such an approach consists of using a water quality simulation model linked with an appropriate optimization model to evaluate management strategies for an impaired watershed. Such a linked methodology will be referred to hereafter as the optimal management model. The use of such an integrated linked methodology has been increasingly popular for water resources management problems and has been successfully used in the past. Some examples of such a linked methodology include the work done by Nicklow and Mays (2000), Muleta (2003), and Dorn (2004). Muleta (2003) provides a listing of several other applications of such a linked methodology in various areas of water resources management such as reservoir management, bioremediation design and groundwater management, and design and operation of water distribution systems. Such a linked approach as shown in Figure 6-1 reduces the complexity and size of the overall optimization framework and provides for the evaluation of several simulation model structures as well as optimization techniques.

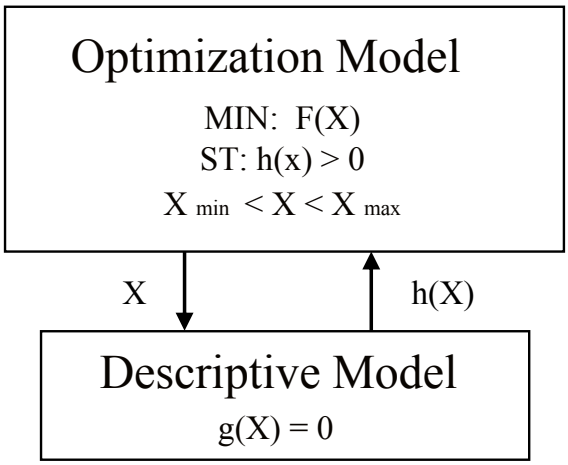


Figure 6-1. General Framework of Linked Methodology

When applied to an urban watershed management and pollution reduction problem, the optimal management model will allow the evaluation of multiple water quality management strategies for the control of point, non-point, and any other sources of pollution in the watershed. The optimal management model can be generally formulated as follows:

Maximize environmental (water quality) and economic (budgetary) benefits for an urban watershed impaired by multiple pollution sources (point, non-point, and other) subject to

1. *Hydrologic and water quality relationships that govern the physical processes modeled in the watershed, and*
2. *Water quality and hydrologic constraints such as regulatory compliance and infrastructure limitations.*

For an urban watershed impaired by point sources (CSOs and SSOs), non-point sources (urban runoff), and other undetermined or unknown sources, the methodology is designed to select optimal management strategies such as volume controls (storage) for CSOs and SSOs, storage for urban runoff such as detention and/or retention facilities, and other site specific controls such as low impact technologies, wastewater treatment technologies, and sewer system rehabilitation techniques.

Two distinct formulations are proposed for the optimal management model. The first one is a water quality-based formulation and the second one is an economic or budget-based formulation. In the water quality-based formulation, the optimal management model evaluates multiple management strategies and selects the optimal strategy that is least-cost and satisfies all water quality objectives. In the budget-based formulation, the optimal management model evaluates multiple management strategies and selects the optimal strategy that minimizes the water quality violation while not exceeding a prescribed project budget.

The methodology developed in this research links a macro-level water quality simulation model with two different optimization techniques for the single objective watershed

management model. The macro-level simulation model is linked in a nonlinear constrained optimization framework to evaluate multiple management strategies leading to the optimal management strategy. The macro-level simulation modeling approach is proposed to represent the hydrologic and/or water quality model for the physical processes occurring in the watershed that are modeled. In theory, three different types of macro-level model structures can be used as described in Chapter 5. These include 1) an implicit inductive model, 2) an explicit inductive model, and 3) a simplified deductive model. While the macro-level approach may limit the accuracy of the model predictability in representing the physical processes modeled, it has several advantages over the use of traditional complex deductive simulation models in the context of an optimal watershed management framework. These include 1) they are relatively simple to develop, 2) they are easy to integrate into the optimal management model, 3) they result in significant time savings when used in the optimal management model, 4) they provide the flexibility of several different model structures and model development techniques for use in the optimal management model. Due to the simplified or macro nature of the simulation model, the resulting optimal management model is proposed for use as a screening tool for evaluating watershed management alternatives. The resulting optimal strategies can be verified or validated with a full blown process-based model, if available.

In the context of the different optimization methods, two different types of optimization techniques are used in the proposed optimal management model namely 1) a GA-based evolutionary optimization method, and 2) a Shuffled Box Complex method of constrained optimization. The use of two different optimization methods will provide for some comparison basis for evaluating the two techniques for application to watershed management problems. In the context of watershed management, two factors make the proposed optimal management model unique when compared to similar work. These include 1) the use of macro-level simulation models for use in the optimal management model, and 2) the use of two different classes or types of optimization techniques in the optimal management model, including a new technique called the Shuffled Box Complex

method. Figure 6-2 is a simplified representation of the optimal management framework proposed in this research.

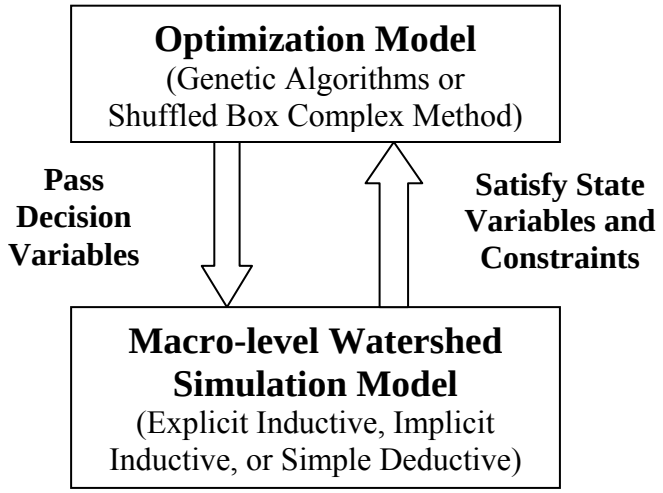


Figure 6-2. Optimal Management Framework

The decision variables in the optimal management formulation as shown in Figure 6-2 above will include management scenarios such as volume controls (storage) for point sources, peak runoff controls, rehabilitation techniques, and any other technologies that can be implemented in an urban watershed for water quality management. Figure 6-3 gives some possible management strategies for an urban watershed. A set of decision variables will consist of the components that make up a possible management strategy (as given in Figure 6-3) that can be implemented in the watershed. These decision variables are sent to the simulation model from the optimization model. The simulation model will evaluate the corresponding response or impact of the system resulting from the particular solution set of decision variables that constitutes a management strategy. The simulation model thus ensures that all implicit system constraints and bound constraints are satisfied. The response of the simulation model is sent back to the optimization model which evaluates the constraints for the model such as violation of water quality or economic constraints. The optimization model continue to send new alternatives in the search for the optimal strategy, the simulation model accept these new alternatives, and the cycle continues until a user specified stopping criterion is satisfied.

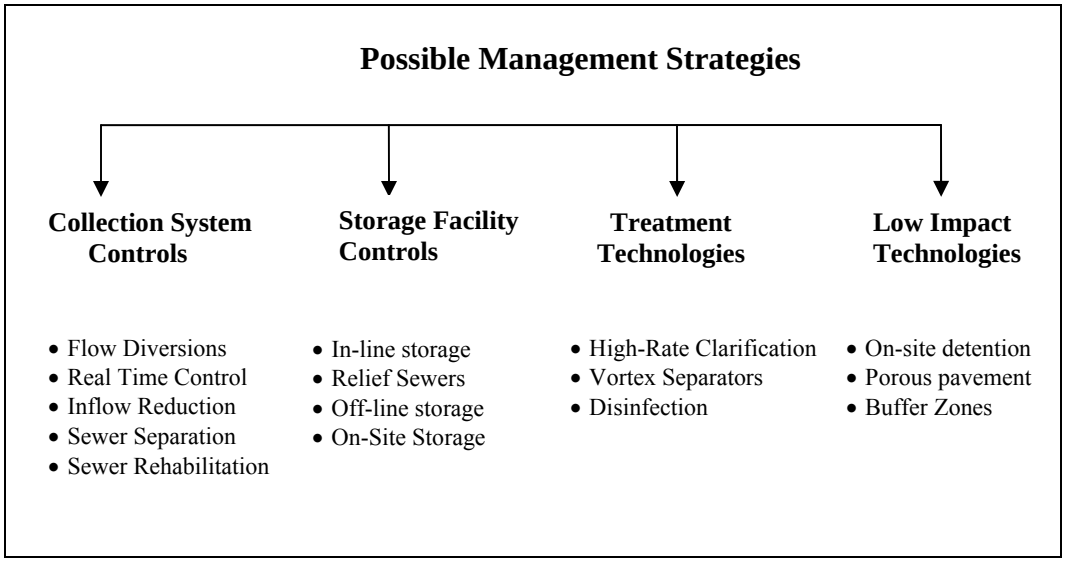


Figure 6-3. Possible Management Strategies for the Optimal Management Model

In GA-based optimal management model, the set of decision variables are coded as genes in a solution chromosome as described in Chapter 2. The suitability or survivability of such chromosome is based on its fitness value, which is directly linked to the objective function(s). Since the optimization is driven by cost, the objective function is a cost function of a management strategy being evaluated. In the Shuffled Box Complex-based optimal management model, the set of decision variables is represented as the vertex of multiple complexes that evolve in the search space. As they evolve, the complexes move towards the constraint boundary and find the optimal solution along the constraint boundary. This method too is driven by cost as the objective function in the search for the optimal solution. In both models, the simulation model is called from the optimization model to evaluate the impact of the proposed strategy on the process or processes being modeled. In GA-based optimization, penalty functions are used to penalize infeasible solutions, while the Shuffled Box Complex method does not require penalty functions.

Every model run starts with an initialization of the optimization model with alternative solution sets. In case of GA-based optimization, an initial population of solution sets is

randomly selected by generating a set of decision vectors within their prescribed explicit bounds. The initial population selected then evolves in the search process and undergoes through the genetic operators of selection, crossover, and mutation as described in Chapter 2. The simulation model is called periodically to evaluate the impact of each solution set on the watershed process or processes (hydrology and water quality). In the Shuffled Box Complex method, the initial solution sets that constitute the vertices of the complexes are selected randomly using the techniques described in Chapter 2. The complexes evolve in the search for the optimal solution, periodically calling the simulation model to evaluate the impact of each solution set on the watershed processes (hydrology and water quality). The complexes are randomly shuffled as they evolve in the search space after a specified number of generations (iterations).

6.5 Water Quality-based Problem Formulation

In the water quality-based approach, the optimal management problem is formulated mathematically as a nonlinear constrained optimization problem to minimize costs while meeting all water quality objectives. The problem will be formulated in a general manner for an urban watershed that has multiple sub-watersheds and three different sources of pollution (point, non-point, and other unknown or undetermined sources). The objective function and associated constraints are given as follows in Equations 6-1 through 6-4.

6.5.1 Objective Function

The objective of the optimal management model for a watershed that is impaired due to point, non-point, and any other unknown or undetermined source is to minimize costs while maintaining acceptable water quality as required by water quality standards. The decision variables that constitute a management strategy (resulting in improvements in the watershed) in the optimization framework can consist of management strategies such as volume controls (storage) for point and non-point sources and any other technologies to rehabilitate infrastructure that is identified as contributing to water quality problems. The volume controls for the point sources may include storage for CSO discharges such

as tunnels to minimize or eliminate the impact of CSO outfalls on the receiving water bodies. Similarly, the volume controls for the non-point sources may include detention/retention storage facilities for treatment and/or removal of various water quality constituents in urban runoff. In the case of infrastructure improvements, possible solutions may consist of sanitary sewer collection system rehabilitation strategies such as sewer lining to reduce wet weather flows and/or replacement of sewers. Mathematically, the objective function may be expressed as given in Equation (6-1).

$$Minimize \quad \psi = \sum_{w=1}^{mw}\left[\left(\sum_{i=1}^{l} C(X_{iw})\right) + \left(\sum_{j=1}^{m} C(Y_{jw})\right) + \left(\sum_{k=1}^{n} C(Z_{kw})\right)\right] \tag{6-1}$$

Where ψ = the total cost of improvements resulting from a management strategy for all the sub-watersheds in an urban watershed, w is the index number for sub-watersheds, nw is the total number of sub-watersheds, i is the index for point sources of pollution, j is the index for non-point sources of pollution, k is the index for other unknown or undetermined sources of pollution, l is the number of point sources in each sub-watershed, m is the number of non-point sources in each sub-watershed, n is the number of unknown or undetermined sources in each sub-watershed, t is the time step used in the model, $X_{i,w}$ is the decision variable for point source control in each sub-watershed, $Y_{j,w}$ is the decision variable for non-point source control in each sub-watershed, $Z_{k,w}$ is the decision variable for unknown or undetermined source control in each sub-watershed, $C(X_{i,w})$ is the cost of point source control decision variable in a sub-watershed, $C(Y_{j,w})$ is the cost of non-point source control decision variable in a sub-watershed, and $C(Z_{k,w})$ is the cost of unknown or undetermined source control decision variable in a sub-watershed.

6.5.2 Constraints

The objective function as described in Equation (6-1) above is subject to three types of constraints: 1) a set of implicit system constraints, 2) a set of implicit bound constraints,

and 3) a set of explicit decision variable bound constraints. These are described as follows.

6.5.2.1 Implicit System Constraints

A macro-level simulation model will be used to satisfy the implicit system constraints that will include all governing hydraulic, hydrologic, and water quality relationships. The decision variables from the optimization model will be passed on to the simulation model which will in turn compute the hydrologic and water quality response of the watershed. Such a response will reflect the effect of a particular management strategy being evaluated by the optimal management model. This is mathematically expressed as given in Equation (6-2).

$$g(X_i, Y_j Z_k) \quad = \quad 0 \qquad \forall\, t \qquad (6\text{-}2)$$

6.5.2.2 Implicit Bound Constraints

The implicit bound constraints include any constraints on the water quality constituent being modeled in the optimal management model. This corresponds to a certain numeric criteria such as greater than a prescribed threshold level as required by the water quality standards. For instance, per Kentucky Water Quality Standards, the dissolved oxygen criterion for aquatic life is 5.0 mg/L (daily average) and 4.0 mg/L (instantaneous minimum) (Kentucky Administrative Regulations Title 401, Chapter 5, Water Quality). For each time step (such as hourly or daily) of the macro-level simulation model, the water quality constituent concentration must be greater than the prescribed water quality standard value. This may be expressed as:

$$h(X_i, Y_j Z_k) \quad \geq \quad WQ_{s\tan dard} \qquad \forall\, w, t \qquad (6\text{-}3)$$

Where w refers to a sub-watershed and *t* refers to the time step in the simulation model.

6.5.2.3 Explicit Decision Variable Bound Constraints

The final set of bound constraints consists of explicit bounds on the decision variables in the optimization model. Mathematically, this may be expressed as given in Equations 6-4 through 6-6.

$$0 \leq X_{iw} \leq X_{\max} \qquad \forall\, i, w \qquad (6\text{-}4)$$

$$0 \leq X_{jw} \leq X_{\max} \qquad \forall\, j, w \qquad (6\text{-}5)$$

$$0 \leq X_{kw} \leq X_{\max} \qquad \forall\, k, w \qquad (6\text{-}6)$$

Where w refers to a sub-watershed and i, j, and k refers to the three types of pollution sources.

6.6 Budget-based Problem Formulation

In the budget-based approach, the optimal management problem is formulated mathematically as a nonlinear constrained optimization problem to minimize the number of water quality violations while satisfying a prescribed project budget. In such a formulation, the total cost of the management strategy evaluated is a constraint while the number of water quality violations constitutes the objective function. The objective function and associated constraints are given as follows in Equations 6-7 through 6-12.

6.6.1 Objective Function

The objective function for a budget-based formulation is to minimize water quality violations while satisfying the cost constraints as prescribed by a project budget. The decision variables that constitute a management strategy in the optimization framework are the same as described in the water quality-based optimal management formulation above. Mathematically, the objective function is expressed as given in Equation (6-7).

$$Minimize \quad \eta \quad = \quad \sum_{w=1}^{nw}\sum_{t=1}^{T}\left[\lambda\left(X_i, Y_j\, Z_k\right)\right]_{tw} \qquad for\, all\, i, j, k \qquad (6\text{-}7)$$

Where η is the number of water quality impairment days, w is the index for sub-watersheds, nw is the total number of sub-watersheds, t is the time step used in the model, i is the index for point sources of pollution, j is the index for non-point sources of pollution, k is the index for other unknown or undetermined sources of pollution, $X_{i,w}$ is the decision variable for point source control in each sub-watershed, $Y_{j,w}$ is the decision variable for non-point source control in each sub-watershed, $Z_{k,w}$ is the decision variable for unknown or undetermined source control in each sub-watershed.

6.6.2 Constraints

The objective function as described in (6-7) above is subject to three types of constraints: 1) a set of implicit system constraints, 2) a set of implicit bound constraints, and 3) a set of explicit decision variable bound constraints.

6.6.2.1 Implicit System Constraints

A macro-level simulation model will be used to satisfy the implicit system constraints that will include all governing hydraulic, hydrologic, and water quality relationships. The decision variables from the optimization model will be passed on to the simulation model which will in turn compute the hydrologic and water quality response of the watershed. Such a response will reflect the effect of a particular management strategy being evaluated by the optimal management model. This is mathematically expressed as given in Equation (6-8).

$$g(X_i, Y_j\, Z_k) \quad = \quad 0 \qquad \forall\, t \qquad (6\text{-}8)$$

6.6.2.2 Implicit Bound Constraints

The implicit constraints include the total cost of a management strategy for the watershed under study. Since this optimal management model is budget based, an upper bound on

total project budget is prescribed and the goal of the optimal management model is to select a management strategy that maximizes the water quality benefits while keeping within the prescribed project budget. This may be expressed as given in Equation (6-9).

$$\sum_{w=1}^{nw}\left[\left(\sum_{i=1}^{l} C(X_{iw})\right) + \left(\sum_{j=1}^{m} C(Y_{jw})\right) + \left(\sum_{k=1}^{n} C(Z_{kw})\right)\right] \leq \Phi \qquad (6\text{-}9)$$

Φ is the prescribed total project budget to be spent in all sub-watersheds that should not be exceeded while maximizing the water quality benefits for the watershed, w is the index number for sub-watersheds, nw is the total number of sub-watersheds, i is the index for point sources of pollution, j is the index for non-point sources of pollution, k is the index for other unknown or undetermined sources of pollution, l is the number of point sources in each sub-watershed, m is the number of non-point sources in each sub-watershed, n is the number of unknown or undetermined sources in each sub-watershed, t is the time step used in the model, $X_{i,w}$ is the decision variable for point source control in each sub-watershed, $Y_{j,w}$ is the decision variable for non-point source control in each sub-watershed, $Z_{k,w}$ is the decision variable for unknown or undetermined source control in each sub-watershed, $C(X_{i,w})$ is the cost of point source control decision variable in a sub-watershed, $C(Y_{j,w})$ is the cost of non-point source control decision variable in a sub-watershed, and $C(Z_{k,w})$ is the cost of unknown or undetermined source control decision variable in a sub-watershed.

6.6.2.3 Explicit Decision Variable Bound Constraints

The final set of bound constraints consists of explicit bounds on the decision variables in the optimization model. Mathematically, this may be expressed as given in Equations 6-10 through 6-12.

$$0 \leq X_{iw} \leq X_{\max} \qquad \forall\, i, w \qquad (6\text{-}10)$$

$$0 \leq X_{jw} \leq X_{\max} \qquad \forall\, j, w \qquad (6\text{-}11)$$

$$0 \leq X_{kw} \leq X_{\max} \qquad \forall\, k, w \qquad (6\text{-}12)$$

Where w refers to a sub-watershed and i, j, k refers to the three types of pollution sources.

6.7 Solution Methodology

The optimal management model as formulated in Sections 6.5 and 6.6 above can be used to evaluate alternative management strategies for a watershed under study. The solution methodology used in both the water quality and budget-based formulations depend on the type of optimization model linked to the macro-level simulation model. As described previously, two types of optimization methods are used in the proposed management model. Thus two solution methodologies are given, each corresponding to the type of optimization method. These two types of methodologies are given in Figure 6-4 (solution methodology for the genetic algorithm-based optimal management model) and Figure 6-5 (solution methodology for the Shuffled Box Complex-based optimal management model). In both cases, the model starts with the initialization of the initial set of solutions or population of solutions. These set of solutions are passed to the macro-level simulation model to evaluate state variables and constraints of the system. The objective function is used to determine the corresponding fitness of the initial set of solutions. In the GA-based optimization, the initial population goes through the genetic operators of selection (based on fitness values), crossover, and mutation to determine the solution set for the next generation (off-springs). The population of solutions thus evolves in this manner from one generation to the next until a user specified stopping criterion is reached or the model is otherwise terminated. As described in Chapter 2, GAs are directly applicable only to unconstrained optimization problems. If a solution set violates any of the implicit bound constraints, a penalty is applied to its fitness value thus degrading the quality of an infeasible solution. Penalty function methods are the most popular methods used for constrained optimization problems using a GA (Yeniay, 2005). These methods transform a constrained problem into an unconstrained problem by imposing a penalty on the infeasible solution. This is done by adding to the objective function value a positive value (penalty) which reduces the fitness value of such infeasible solutions (Yeniay, 2005). This decreases the chances of the solution to have a significant impact on the offspring solutions as they evolve in future generations. Both static and dynamic penalties can be applied when using GAs for constrained optimization (Sarker et al. 2002). In this research, static penalty functions were used to penalize infeasible solutions in the GA search process. In static penalty methods, several levels of violation are

created for each constraint, and for each level of violation and each constraint, a penalty coefficient is created. Higher levels of violation can thus be penalized more than lower levels of violation. In most cases, the optimization model is terminated when there is no further improvement in the global optimal solution obtained in the GA search process.

In the Shuffled Box Complex-based optimization, a single feasible initial solution is generated that satisfies all system state equations as well as implicit and explicit bound constraints. The model then generates additional initial solution sets in a sequential manner using random numbers and the explicit bounds of the decision variables. These initial solution sets are used to form the vertices of the complexes. The solution sets are partitioned into a specified number of complexes with each vertex of a complex representing a feasible solution (set of decision variables representing a particular watershed management strategy). Each complex then evolves in the search space through the process of complex expansion and contraction as explained in Chapter 2. Each successful expansion or contraction results in the worst solution in the complex being replaced by a new solution set and thus represent a new generation. After a certain number of specified generations, the solution sets in individual complexes are shuffled randomly and re-assigned to individual complexes. After the shuffling, each complex is set to evolve again in the search space. The model is terminated after a specified number of generations (iterations) for each complex and corresponding number of shuffling operations. The termination usually occurs when the complexes collapse into the centriod and there is no further improvement in successive generations.

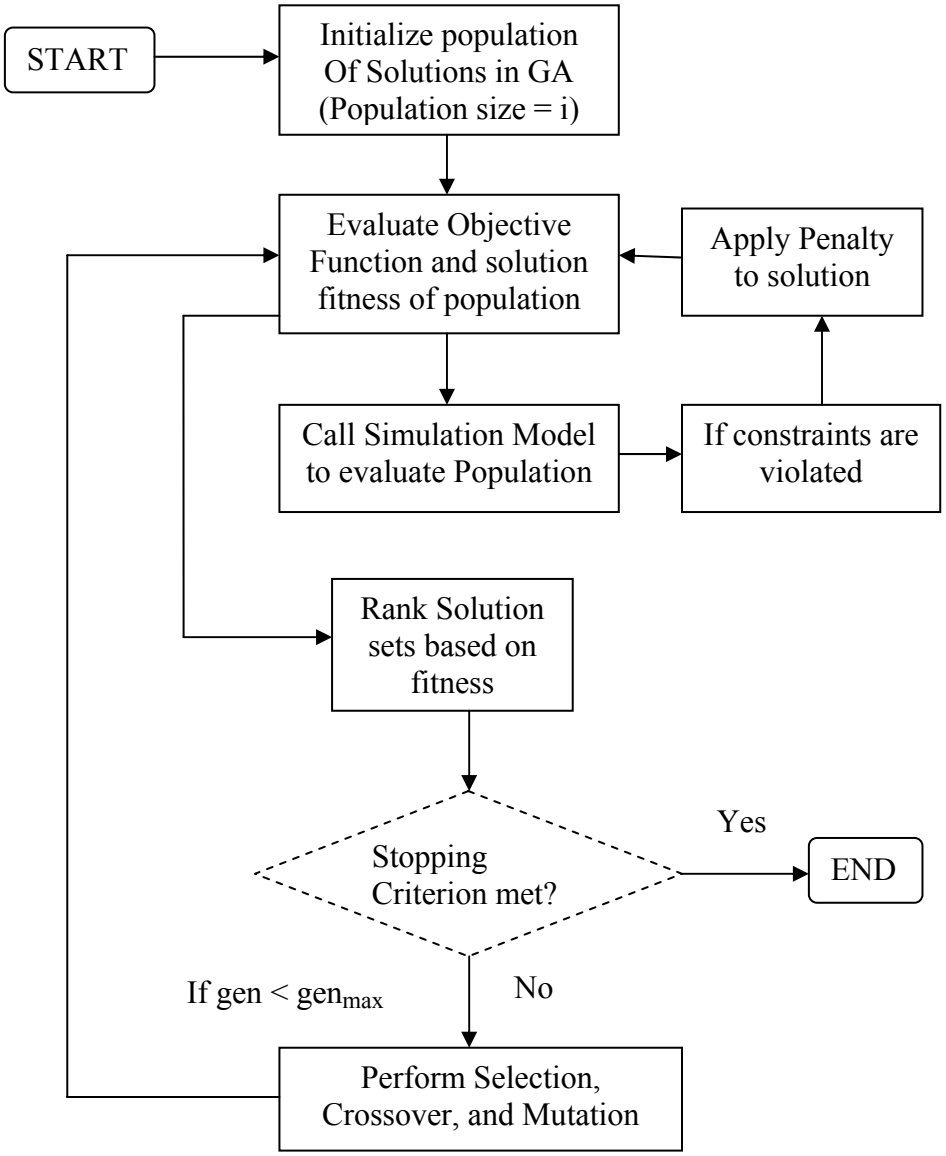


Figure 6-4. Schematic of GA-based Optimal Management Model

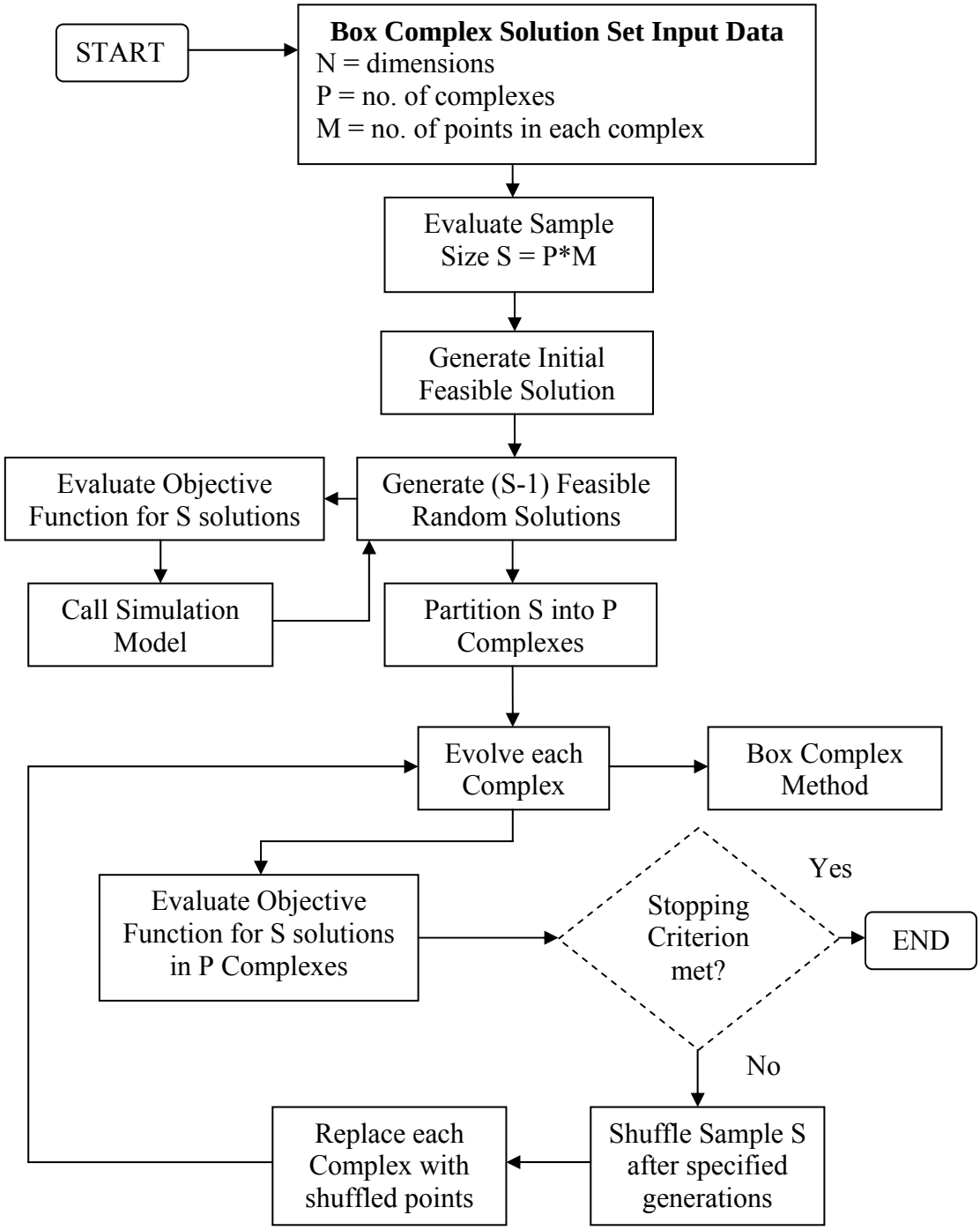


Figure 6-5. Schematic of the Shuffled Box Complex-based Optimal Management Model

CHAPTER 7

EXAMPLE APPLICATION OF THE OPTIMAL MANAGEMENT MODEL

7.1 Introduction

The optimal management model formulations described in Chapter 6 were applied to the problems faced by environmentalists, local, state, and federal regulatory authorities, and general citizens of the Beargrass Creek watershed in Louisville, Kentucky. Beargrass Creek watershed (one of the 9 watersheds in Jefferson County, Kentucky) is a highly complex urban watershed with a total drainage area of approximately 61 square miles. The watershed consists of three distinct streams representing three sub-watersheds, and is impaired due to low dissolved oxygen and/or nutrient enrichment, and pathogens (Figure 7-1). This watershed provides for an excellent application of the optimal management model as it is urban, consists of distinct sub-watersheds, and is impaired by multiple sources of pollution including point and non-point sources. Five segments of the Beargrass Creek are on the State of Kentucky's 303(d) list of impairment and currently pathogens TMDL and dissolved oxygen/nutrient TMDL are being developed for the watershed (KDOW, 2003). A comprehensive water quality monitoring program is currently in place to collect pertinent data for the watershed. A suite of hydrologic and water quality models are also currently being developed to characterize the hydrologic and water quality response in the watershed. The sources of pollution include storm water runoff as well as wet weather discharge from numerous CSOs and SSOs. There are approximately 37 SSOs, 57 CSOs, and 1000 storm water discharge points in the watershed. In the example application, the optimal management model will be used to evaluate water quality management strategies to improve the dissolved oxygen in the impaired segments of the watershed.

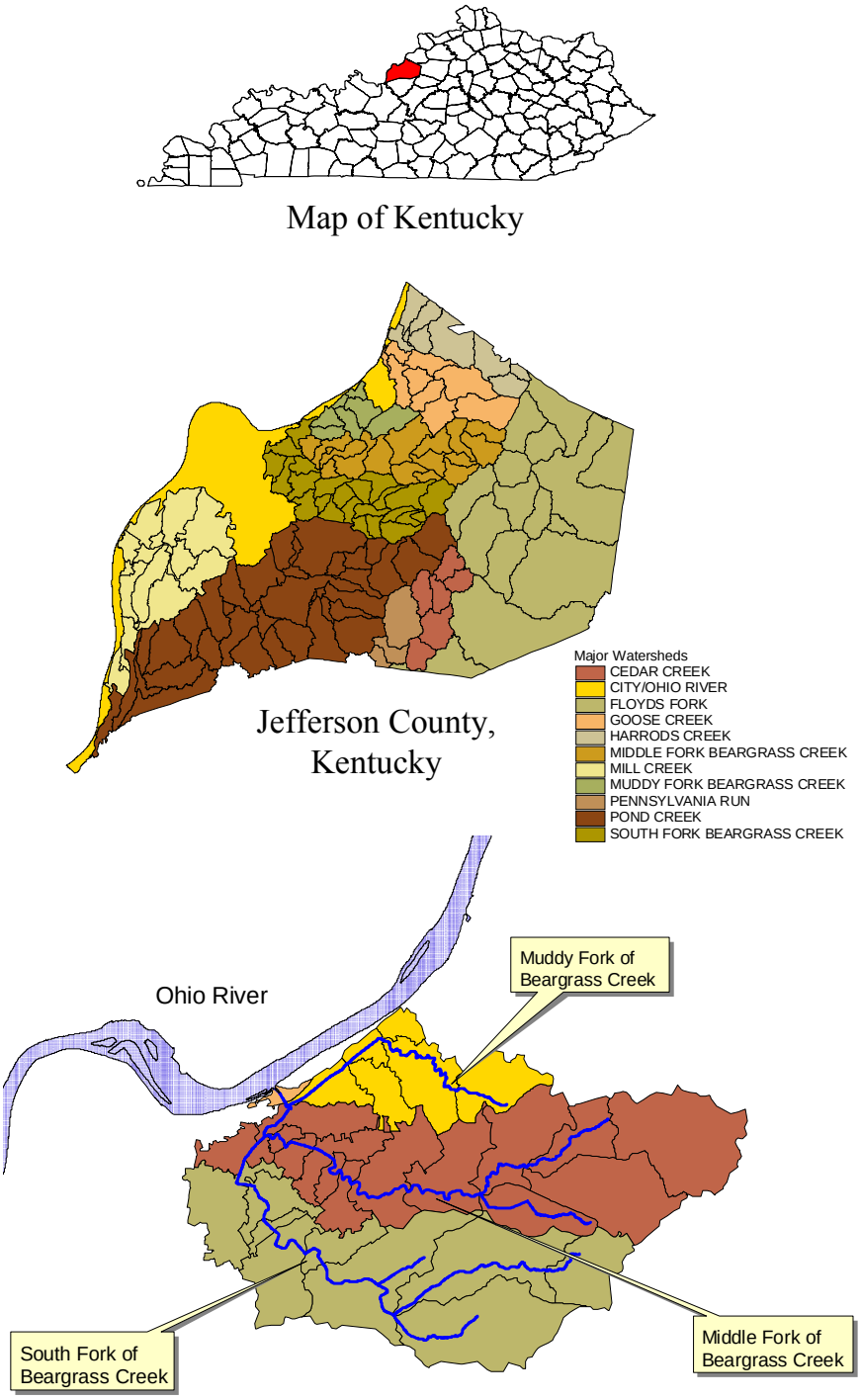


Figure 7-1. Beargrass Creek Watershed, Louisville, Jefferson County, Kentucky

The Commonwealth of Kentucky filed a civil suit against MSD in state court in February, 2004 for unlawful discharge of untreated sewage and overflows of combined sewage into the Ohio River and its tributaries totaling billions of gallons each year. The U.S. Department of Justice, U.S. Environmental Protection Agency, and Commonwealth of Kentucky's Environmental and Public Protection Cabinet (EPPC) jointly signed a consent decree on April 25, 2005 for a comprehensive Clean Water Act settlement with the Louisville and Jefferson County Metropolitan Sewer District (MSD). The settlement requires that MSD will make extensive improvements to its sewer systems to eliminate unauthorized discharges of untreated sewage and to address problems of overflows from sewers that carry a combination of untreated sewage and storm water at a cost likely to exceed $500 million (U.S. Department of Justice, 2005). This is a challenging task and would require an effective management tool to evaluate least-cost management strategies to achieve water quality goals as agreed upon in the consent decree.

7.2 Beargrass Creek Watershed, Louisville, Kentucky

The optimal management model will be used to evaluate management strategies to improve the dissolved oxygen in each of the contributing sub-watersheds of Beargrass Creek watershed and obtain BOD load reductions in the most cost-effective manner while satisfying water quality objectives. The following sections will give a summary of the regulatory history of Jefferson County, Louisville, Kentucky, a detailed description of the Beargrass Creek watershed and the problems that need to be addressed through water quality modeling and management.

7.2.1 Regulatory History of Jefferson County

The Louisville and Jefferson County Metropolitan Sewer District (MSD) was created on July 9, 1946 after which it took over the city's sewer system and allowed it to expand its service area throughout Jefferson County. MSD provides sanitary sewer, storm water drainage, and flood protection services to over 200,000 customer accounts. All capital projects relating to sanitary sewers, storm sewers, and flood control structures in all nine

watersheds in Jefferson County are managed by MSD. MSD is also responsible for overall management of these watersheds as it relates to restoring water quality impairments resulting from natural or man-made activities in the watersheds

MSD is responsible for the operation and management of three different types of programs relating to capital infrastructure, water quality, and watershed management. These include the MS4 (Municipal Separate Storm Sewer System) program, the CSO (Combined Sewer Overflows) program, and the SSO (Sanitary Sewer Overflows) program. The programs are briefly described below:

7.2.1.1 MS4 Program

The purpose of the Municipal Separate Storm Sewer System (MS4) program is to manage the separate storm sewer system and to maintain and enhance water quality in Jefferson County. The purpose is also to protect and promote the public health, safety and welfare by preventing the introduction of harmful materials into the separate storm sewer system (Louisville-Jefferson County MSD website, 2005a).

7.2.1.2 CSO Program

The Morris Forman Wastewater Treatment Plant (MFWTP) KPDES Permit required that MSD develop and implement a Combined Sewer Overflow (CSO) Abatement Program. The objective of the CSO Abatement Program is to reduce the pollutant loads caused by CSOs on receiving streams through compliance with the EPA CSO Control Policy. The initial phase of the program began in early 1991 and culminated in the development of a Combined Sewer Operational Plan (CSOP). Since that time, yearly updates to the original CSOP have been prepared.

The EPA CSO Control Policy, published in 1994, provided guidance on coordinating the planning, selection and implementation of CSO controls that meet the requirements of the Clean Water Act. The policy contained provisions for developing appropriate, site-

specific NPDES permit requirements for combined sewer systems that overflow as a result of wet weather events. The policy established two main objectives for permittees: implementation of the Nine Minimum Controls (NMCs), and the development and implementation of a CSO Long-Term Control Plan (LTCP).

The nine minimum CSO controls as outlined by the Environmental Protection Agency (EPA, 1995) are given as follows:

1. Proper operation and regular maintenance programs for the sewer system and CSO outfalls.
2. Maximum use of the collection system for storage.
3. Review and modification of pretreatment requirements to ensure that CSO impacts are minimized.
4. Maximization of flow to publicly owned treatment works for treatment.
5. Elimination of CSOs during dry weather.
6. Control of solid and floatable materials in CSOs.
7. Pollution prevention programs to reduce contaminants in CSOs.
8. Public notification to ensure that the public receives adequate notification of CSO occurrences and CSO impacts.
9. Monitoring to effectively characterize CSO impacts and the efficacy of CSO controls.

The intent of the NMCs is to secure the prompt implementation of control measures that will at least partially control wet weather CSO discharges. Per the CSO Control Policy, MSD's NMCs were implemented on January 1, 1997. Selection and implementation of actual control measures was based on consideration of the specific combined sewer system and in many cases may address more than one of the NMCs.

The policy also directed the permittee to develop and implement a LTCP based on characterization, monitoring and modeling of the combined sewer system. The plan

considers the site-specific nature of CSOs and gives highest priority to controlling overflows in sensitive areas (Louisville-Jefferson County MSD website, 2005b).

7.2.1.3 SSO Program

The Sanitary Sewer Overflow (SSO) program is MSD's centralized program for managing the investigation, prioritization and rehabilitation of the separate sanitary sewer system in order to abate sanitary sewer overflows and basement backups. This program represents MSD's proactive approach toward eliminating excess inflow and infiltration (I/I) from the separate sanitary collection system. MSD's SSO Program has the following goals:

- Eliminate and/or reduce the frequency/volume of recurring SSOs caused by excessive I/I.
- Eliminate basement flooding caused by sewer backup as a result of excessive I/I.
- Reduce MSD expenditures to construct, maintain, and operate sewage collection and treatment systems impacted by existing I/I.
- Assure compliance with the Kentucky Division of Water (KDOW) regulations governing sanitary lateral extensions and wastewater treatment plant upgrades (Louisville-Jefferson County MSD website, 2005c).

7.2.2 Water Quality Management in Jefferson County

MSD employs an aggressive approach to investigate, evaluate and develop solutions to the water quality issues facing Jefferson County, Kentucky. Specific programs initiated by MSD in this regard are discussed as follows.

7.2.2.1 MSD's Wet Weather & Water Quality (WWWQ) Program

Since 1999, the Louisville Jefferson County Metropolitan Sewer District (MSD) has been in the process of transitioning from a programmatically-driven approach to one that is

more water quality-driven. In the past, the MS4, CSO, and SSO programs (described in the previous section) were reported and managed separately within MSD. To attain the goal of a water quality-based program, MSD has had to redefine goals and reorganize departments. In 2002 the Wet Weather & Water Quality (WWWQ) program was started, with the responsibility of combining the MS4, CSO, SSO and water quality programs into one comprehensive program. The creation of the WWWQ program allows for a more effective integration of MSD's regulatory responsibilities across departmental boundaries. The responsibilities of the WWWQ Team stretch across all nine watersheds in Jefferson County (Figure 7-1) with an ultimate goal of improving the water quality in these watersheds (Louisville-Jefferson County MSD website, 2005d).

7.2.2.2 Watershed Management Approach

Through the implementation of a Wet Weather & Water Quality (WWWQ), MSD employs an aggressive approach to investigate, evaluate and develop solutions to the wet weather and water quality issues facing Jefferson County, Kentucky. The sources of water quality impairment are multi-faceted. MSD's approach is that of watershed management, in which all sources of impairment are evaluated simultaneously to determine real solutions to real problems and to obtain the ultimate goal – stream water quality enhancement (Louisville-Jefferson County MSD website, 2005d).

In the watershed management approach, MSD decided to break the strategic plan of overall water quality improvement into more manageable pieces. It was decided to use a five year planning window consistent with MSD's capital budgeting process. The mission statement was then refined for this first five-year period. Specifically, it called for the development and implementation of a sustainable strategic process for water quality management within the wet weather programs. The process selected was called the Resource Management Process (RMP). The goal for this process was to be transferable and applicable to all county watersheds (Louisville-Jefferson County MSD website, 2005d).

This process sets the foundation for water quality-based decision making and will be utilized to integrate programs, as well as manage resources, on a watershed basis. This process should allow MSD to prioritize the Capital Improvement Program (CIP) using criteria that reach beyond just regulatory requirements, taking into account environmental benefit, habitat, biodiversity, and community livability goals. The RMP is cyclic because the process of watershed management is dynamic. Conditions and priorities change; therefore, the community needs a process that is responsive and adaptive to change. The cyclic process chosen ensures that CIP decisions will be periodically reviewed and adapted as necessary to optimize resources (Louisville-Jefferson County MSD website, 2005d).

Selection of a Watershed as the pilot implementation area

Of the 9 watersheds within Metro Louisville (Figure 7-1), the Beargrass Creek watershed was selected as the pilot implementation area for which a comprehensive water quality assessment, modeling, and management was to be performed. This watershed has an area of approximately 61 square miles and contains about 148 streams miles. The Beargrass Creek Watershed contains three sub-watersheds namely South Fork, Middle Fork, and Muddy Fork watersheds. The watershed is approximately 38% impervious area with a land use breakdown of 44% residential, 5% industrial, 20% commercial, 15% public, 4% parks, and 12% undeveloped. It contains 57 CSOs, 37 SSOs and 1,000 storm water outfalls.

MSD has developed the Beargrass Creek Water Quality Model (BCWQM). This tool utilizes a suite of hydraulic, hydrologic, and water quality simulation computer models (specifically, they use HSPF, XP-SWMM, and CEQUAL2-RV1) to predict the potential benefits for the watershed for various alternative scenarios, including combinations of alternatives. This predictive tool is currently under development and upon completion will be utilized to develop program priorities and project scheduling.

The 2002 Kentucky 303(d) list classifies all three forks within Beargrass Creek as not meeting the designated-use criteria for Primary Contact Recreation and Aquatic Life due

to pathogens and organic enrichment/dissolved oxygen. Per the Clean Water Act (CWA) provisions for establishing section 303(d) list priority ranking of impaired waters and to establish total maximum daily loads (TMDLs) for such waters, dissolved oxygen and pathogen TMDLs are scheduled to be completed in December 2006. These TMDLs will rely heavily on the monitoring network and BCWQM developed by MSD. The Kentucky Division of Water (KDOW), in partnership with the University of Kentucky and MSD, will develop the TMDLs with the financial assistance of a USEPA Region IV grant. The TMDL reports will be submitted to EPA Region IV for approval.

The next step will be to use the TMDL in concert with the Beargrass Creek stakeholder group and the RMP to develop a Watershed Plan that minimizes or eliminates the discharge of wet weather pollutants to Beargrass Creek. The process will serve to define the problems and describe policies, programs, and activities necessary to rehabilitate and manage the watershed. The intent is to use the process developed for Beargrass Creek as a model for the other watersheds across the county.

7.2.3 Description of the Beargrass Creek Watershed

The Beargrass Creek watershed drains approximately 61 mi^2 (38,970 acres) of eastern Jefferson County located in north-central Kentucky, bordering and draining into the Ohio River. The Beargrass Creek watershed is comprised of three tributary sub basins: South Fork (27.0 mi^2), Middle Fork (25.1 mi^2), and Muddy Fork (8.9 mi^2) as shown in Figure 7-2. The two southern tributaries, South and Middle Forks join together to form the lower reaches of the Beargrass Creek, and Muddy Fork then joins the flow from the combined South Fork and Middle Fork prior to entering the Ohio River (Jarrett et al. 1998; Jarrett, and Saffran, 1999).

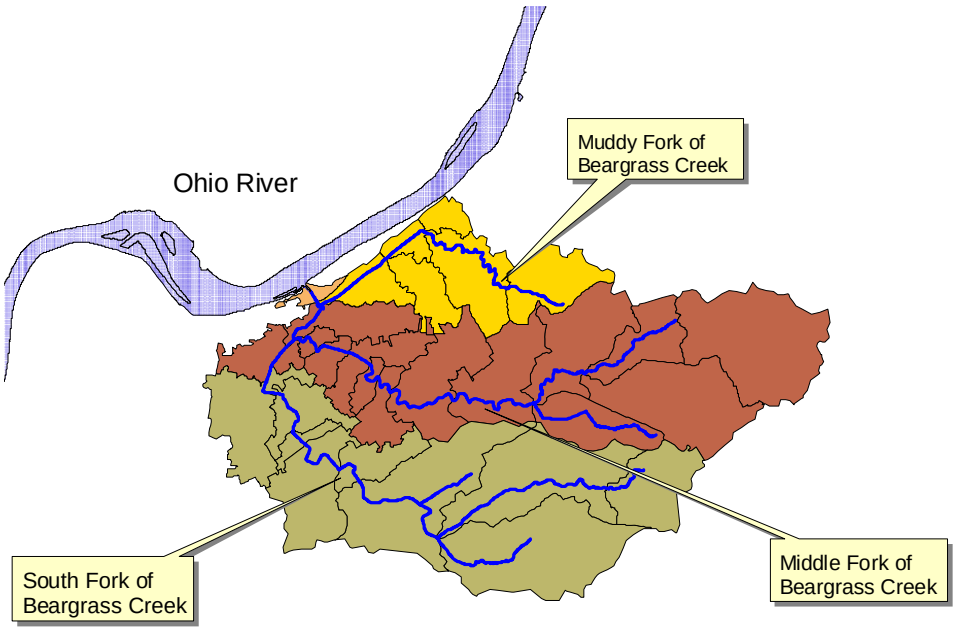


Figure 7-2. Three tributaries of the Beargrass Creek Watershed

Elevation in the Beargrass Creek watershed ranges from 420 feet, along the stream channel at the northwestern extent of the watershed, to 748 feet above mean sea level at the eastern extent of the Middle Fork sub basin. The headwaters drain Silurian age dolomite, shale, and minor amounts of limestone. The creek cuts into Devonian age limestone and shale before flowing into the Ohio River. A more detailed description of the basins can be found in Evaldi and Moore (1992). Land use in the basins varies from single family residential to light industrial. The dominant land use in all three sub basins is single-family residential, followed by paved (impervious) surfaces (roads and parking lots), parks, and cemeteries (Table 7-1).

Table 7-1. Land use in Beargrass Creek Watershed

Land Use	South Fork		Middle Fork		Muddy Fork	
	Area (sq-mi)	Percent (%)	Area (sq-mi)	Percent (%)	Area (sq-mi)	Percent (%)
Single-family residence	12.6	46.7	11.0	43.8	5.00	56.0
Multiple-family residence	1.3	4.7	1.5	5.8	0.60	6.7
Commercial	2.1	7.6	2.2	8.7	0.30	3.0
Industrial	1.1	4.1	0.3	1.0	0.05	0.6
Churches, schools, non-commercial	1.6	5.8	1.5	6.1	0.30	3.5
Parks, cemeteries, public open space	2.6	9.8	2.8	11.2	0.80	8.9
Vacant or undeveloped	1.7	6.2	2.5	9.8	0.90	0.1
Roads and other paved areas	4.1	15.1	3.4	13.6	1.10	10.0

Most of the watershed is sewered with separate sanitary and storm sewers (27,906 acres, 72%). The dense commercial central business district is drained mainly by a complex system of combined sanitary and storm sewers, with few open channels and several miles of concrete channels. A section of the concrete channel in the South Fork tributary of the Beargrass Creek is given in Figure 7-3. Due to the intensity of development within this watershed, streams in the Beargrass Creek watershed are true urban streams. A very high percentage of this watershed is impervious. In addition, there are 57 combined sewer overflows (CSOs) and 37 sanitary sewer overflows (SSOs) in the area. This combination results in moderate to high nutrient levels. Fecal coliform populations exceed pollution standards almost two thirds of the time. Fast moving storm water scours the stream banks, causing erosion, sedimentation, siltation, and resulting in the decline of water quality and habitat quality. Physical pressures, high water fluctuations during storm events, and microbiological effects result in severe impacts on both habitat and the biological communities in the streams.

Figure 7-3. Section of concrete channel in South Fork of Beargrass Creek

Overall water quality impacts to the streams in Beargrass Creek watershed are considered moderate to severe. Impacts here are also highly variable, depending on the flow rate. No quick fixes will help reduce the impacts to this urban watershed. Solutions to the issues facing the Beargrass Creek watershed will have to be long term. Better water quality and quantity management requires the reduction of CSO and SSO discharges, as well as addressing non-point source pollution issues. Re-vegetation of stream banks and modification of stream channels to produce reaeration zones will help to improve both habitat and water quality.

7.2.3.1 South Fork of Beargrass Creek Watershed

The South Fork of Beargrass Creek Watershed is approximately 27 square miles, and includes a portion of metropolitan Louisville. South Fork of Beargrass Creek begins above Bardstown Road area and flows through the northeastern section of downtown Louisville before emptying into the Ohio River. Several miles of this stream have been enclosed in concrete U-shaped channels.

7.2.3.2 Middle Fork of Beargrass Creek Watershed

The Middle Fork of Beargrass Creek watershed is approximately 25 square miles, and includes a section of metropolitan Louisville. The Middle Fork begins in the Middletown

area, runs through Cherokee and Seneca Parks, and later empties into the South Fork of Beargrass Creek.

7.2.3.3 Muddy Fork of Beargrass Creek Watershed

The Muddy Fork of Beargrass Creek Watershed is approximately 9 square miles, and includes a section of metropolitan Louisville. Muddy Fork runs along the Ohio River emptying into the South Fork of Beargrass Creek. It also receives backwater from the river.

7.2.4 Water Quality Conditions and Impairments in Beargrass Creek Watershed

Beargrass Creek has several stream segments on the State 303(d) list for aquatic life and recreational impairment. These streams are listed for impairment due to pathogens and low dissolved oxygen and/or nutrient impairment. Since this research will focus on the dissolved oxygen impairment, only a description related to dissolved oxygen impairment is given as follows.

7.2.4.1 Dissolved Oxygen Impairment

The Kentucky Surface Water Standards include numerical criteria for dissolved oxygen for the protection of aquatic life in warm water habitats. The Surface Water Standards specify that dissolved oxygen shall be maintained at a minimum concentration of 5.0 milligrams per liter (mg/l) daily average; the instantaneous minimum shall not be less than 4.0 mg/l in warm-water (Kentucky Administrative Regulations Title 401, Chapter 5, Water Quality). Low dissolved oxygen is a significant water quality problem in the Beargrass Creek watershed. A comprehensive water quality sampling program is in place for the watershed and DO measurements are recorded at 20 continuous monitoring sites throughout the watershed (Figure 7-4). These readings are taken every 15 minutes and can be compiled into hourly and daily data for a study period.

In 1999 a study was conducted to determine the factors that controlled dissolved oxygen concentrations in the Middle Fork and South Fork Beargrass Creek. Ruhl and Jarrett (1999) identified the environmental processes that most affect DO concentrations during base flow periods in the lower reaches of Middle Fork and South Fork Beargrass Creek. These reaches are affected by inputs from combined sewer overflows. The results of the study indicated that algal production, stream flow, reaeration, and sediment oxygen demand (SOD) are the factors that most affect net production and depletion of DO in the lower reaches of the Middle Fork and South Fork Beargrass Creek. More recent data suggest that organic load from CSO discharges may be a potential cause for some of the chronic dissolved oxygen crashes after a major storm event. Overall, it is hypothesized that there are three sources of pollution that can cause the dissolved oxygen deficit in the Beargrass Creek watershed. These include 1) point sources such as CSO discharges, 2) non-point sources such as organic load in urban storm water runoff, and 3) an unknown and undetermined source that may include other suspected sources of organic load such as leaking sewers resulting in ex-filtration of BOD load onto the banks of streams.

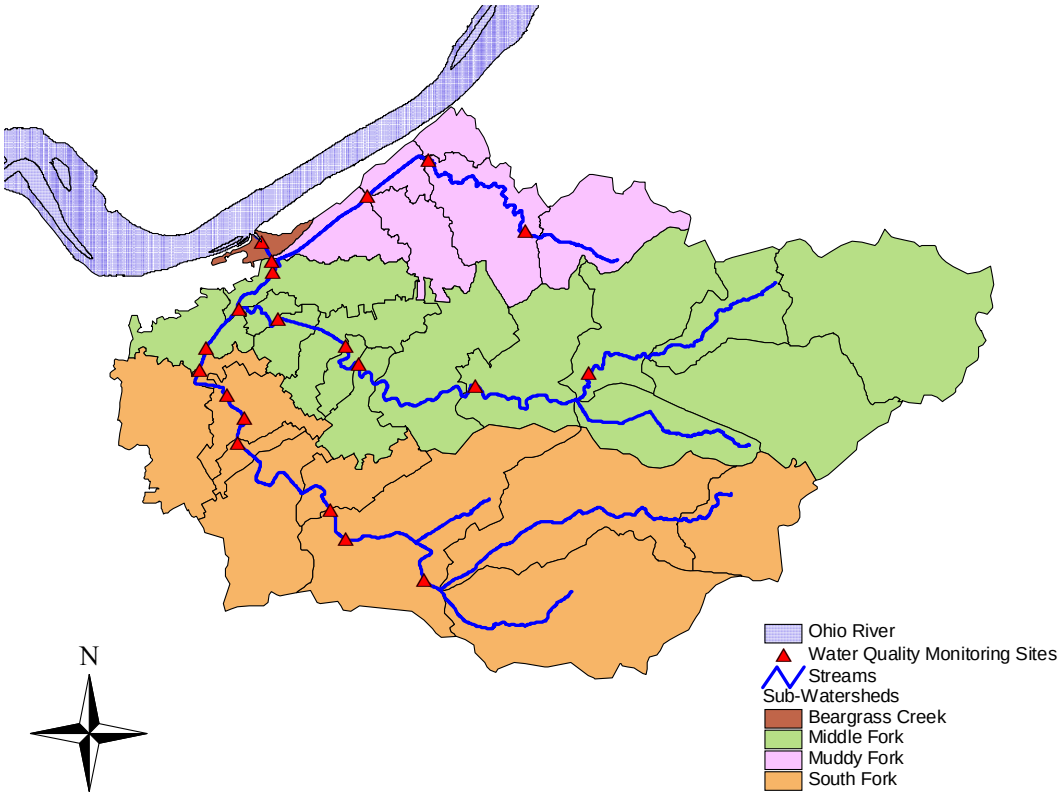


Figure 7-4. Continuous Monitoring Stations in Beargrass Creek Watershed

7.2.4.2 303(d) Listings for Beargrass Creek Watershed

The impairments in the Beargrass Creek Watershed have been formally identified on the 303(d) List of Waters for Kentucky using data collected by the Louisville and Jefferson County Metropolitan Sewer District. (KDOW, 2003). The water bodies that are listed on 2002 303(d) List due to nonsupport of designated uses are given in Figure 7-5.

Impairment #1 - Beargrass Creek of Ohio River
River Mile 0.0 to 1.6 (Segment Length: 1.6 miles)
Impaired Use: Aquatic Life (Nonsupport)
Pollutant of Concern: Metals, Organic Enrichment/Low DO
Suspected Sources: Municipal Point Sources, Combined Sewer Overflows, Urban Runoff/Storm Sewers

Impairment #2 - Middle Fork Beargrass Creek
River Mile 0.0 to 2.3 (Segment Length: 2.3 miles)
Impaired Use: Aquatic Life (Nonsupport), Swimming (Nonsupport)
Pollutant of Concern: Organic Enrichment/Low DO, Habitat Alteration, Metals (Cadmium), Pathogens
Suspected Sources: Combined Sewer Overflows, Urban Runoff/ Storm Sewers, Hydromodification (Channelization).
The most recent information shows that Middle Fork is no longer impaired by metals, but the data are limited.

Impairment #3 - Middle Fork Beargrass Creek
River Mile 2.3 to 15.2 (Segment Length: 12.9 miles)
Impaired Use: Swimming (Nonsupport), Aquatic Life (Partial Support)
Pollutant of Concern: Pathogens, Metals (Cadmium)
Suspected Sources: Industrial Point Sources, Municipal Point Sources, Urban Runoff/Storm Sewers, Land Disposal, Combined Sewer Overflows, Sanitary Sewer Overflows

Impairment #4 - South Fork Beargrass Creek
River Mile 0.0 to 2.7 (Segment Length: 2.7 miles)
Impaired Use: Aquatic Life (Partial Support), Swimming (Nonsupport)
Pollutant of Concern: Metals (Cadmium), Pathogens, Organic Enrichment/Low DO
Suspected Sources: Municipal Point Sources, Urban Runoff/Storm Sewers, Land Disposal, Combined Sewer Overflows, Sanitary Sewer Overflows

Impairment #5 - South Fork Beargrass Creek
River Mile 2.7 to 14.6 (Segment Length: 11.9 miles)
Impaired Use: Swimming (Nonsupport), Aquatic Life (Partial Support)
Pollutant of Concern: Pathogens, Organic Enrichment/Low DO
Suspected Sources: Municipal Point Sources, Urban Runoff/Storm Sewers, Land Disposal, Combined Sewer Overflows, Sanitary Sewer Overflows

Figure 7-5. List of Water Quality impairments in Beargrass Creek Watershed

7.3 Optimal Management Model for Beargrass Creek Watershed

The optimal management model described in Chapter 6 was applied to Beargrass Creek watershed to evaluate management strategies for improving the dissolved oxygen impairment in the watershed. Such an optimal management model would require a macro-level watershed simulation model linked with an optimization model. Both the GA-based and Shuffled Box Complex-based optimization techniques will be used in the optimal management model for Beargrass Creek watershed. In selecting an approach for the macro-level simulation model of the process in hand (dissolved oxygen), three possible model structures were evaluated. These are summarized as follows:

1. Explicit Inductive Model

   Multiple explicit dissolved oxygen inductive models were developed using artificial neural networks (ANNs) and evaluated for use in the optimization framework. These included hourly and daily dissolved oxygen models as described in Chapter 5. The approach was not viable due to a failure to establish a reasonably accurate cause-and-effect relationship between input (independent) and output (dependent) variables of the inductive models. This can be attributed to the unavailability of sufficient raw data for model development or the fact that the raw data used in model development may have been erroneous.

2. Implicit Inductive Model

   Another alternative was to develop implicit inductive models based on the output from a calibrated complex deductive suite of models for the watershed under study. This alternative was not viable as the complex deductive models for the Beargrass Creek watershed are currently in the development phase and have not yet been calibrated for water quality.

3. Simple Deductive Model

   The third and last alternative was to develop a simple and conceptual deductive model that is calibrated with observed data obtained during data collection. Such a deductive approach can serve as an effective substitute to a complex deductive model,

particularly for evaluating management scenarios on a macro level. Once a particular optimal solution or set of solutions are selected, a more complex and detailed deductive model can be used to validate such alternatives. This approach was selected to demonstrate the application of the optimal management model to the Beargrass Creek watershed. The inverse loading dissolved oxygen model based on Streeter-Phelps equations was developed for Beargrass Creek watershed (as described in Chapter 5) and used as the water quality simulation model in the optimal management model for this application. The model is referred to as an inverse loading model because of its novel approach of first backing out an effective BOD concentration based on the observed DO deficit (using raw data collected), and then disaggregating the BOD load (flow and concentrations) resulting from various pollution sources (point, non-point, and unknown sources). After disaggregating the BOD loads, the model is solved in the forward direction to compute the DO time series for the contributing watersheds.

The objective of the optimal management model for Beargrass Creek watershed is to minimize costs while satisfying the dissolved oxygen (DO) criteria (above a certain threshold value as required by Kentucky State water quality standards). The watershed is impaired due to low DO and/or nutrient enrichment. The explicit inductive ANN-based DO models developed for the watershed (as described in Chapter 5) led to the assumption that organic (BOD) loads were responsible for the DO crashes observed in the raw data. In the context of the organic loads, three different types of pollution sources were identified as contributing organic (BOD) loads in the receiving streams. These include point sources (CSO discharges), non-point sources (urban runoff), and an unknown source that was assumed to be linked to leaking sewers along the stream banks. The decision variables that constitute a particular management strategy evaluated in the proposed optimization framework consists of 1) volume controls for point sources, 2) volume controls for non-point sources, and 3) a strategy to rehabilitate leaking sewer lines along the stream to minimize or eliminate leakage of organic matter (measured as BOD in mg/L) onto the banks of the stream. The volume controls for the point sources include storage (deep tunnels) for CSO discharges to minimize or eliminate organic

matter from CSO outfalls into the stream. Similarly, the volume controls for the non-point sources include storage facilities (detention/retention basins) for treatment and/or removal of organic matter carried in urban runoff. Thus for each of the three forks of the Beargrass Creek watershed, one point source decision variable and one non-point source decision variable is used in the optimization framework. In the case of sewer rehabilitation strategy for each of the three forks, the decision variables consist of lengths of sewers of different diameters along the stream reach that would need to be lined. There are four classes of sewers (classified based on the diameter of the sewer line) in the South Fork, three classes in the Middle Fork, and three in the Muddy Fork. In total, there are 16 decision variables in the optimal management model formulation including six for the South Fork, and five each for the Middle and Muddy Fork sub-watersheds of Beargrass Creek watershed. These are given in Figure 7-6 below.

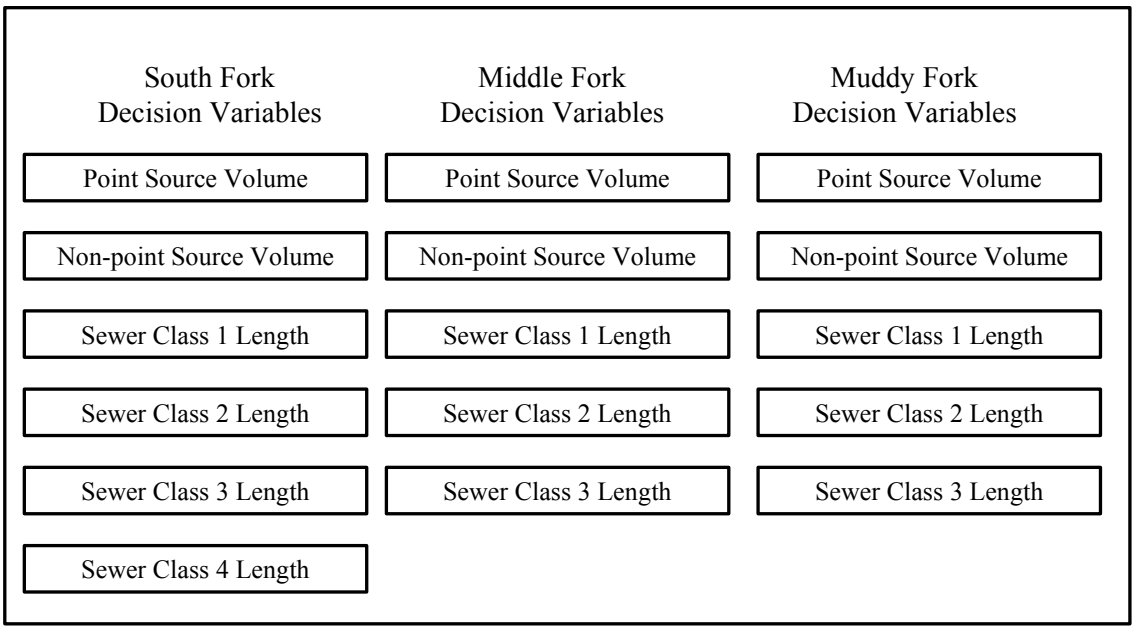


Figure 7-6. Decision variables in the optimal management formulation

The proposed optimal management model for Beargrass Creek watershed consist of two distinct formulations namely 1) a water quality based formulation, and 2) a budget based formulation. In both cases, the optimal management problem is formulated

mathematically as a nonlinear constrained optimization problem. The two optimal management model formulations and associated results are given as follows.

7.4 Water Quality-based Optimal Management Model

In the water quality-based formulations, the objective is to minimize costs and achieve all water quality goals. In such a formulation, the objective function and the associated constraints are discussed below.

7.4.1 Objective Function

Mathematically, the objective function may be expressed as:

$$Minimize \quad \psi = \sum_{w=1}^{3}\left[\left(C(X_{iw})\right) + \left(C(Y_{jw})\right) + \left(\sum_{k=1}^{n} C(Z_{kw})\right)\right] \tag{7-1}$$

Where ψ = the total cost of improvements resulting from a management strategy for all the three sub-watersheds, w is the index number for each sub-watersheds, i is the index for point sources of pollution , j is the index for non-point sources of pollution, k is the index for other unknown or undetermined sources of pollution, n is the number of unknown or undetermined sources in each sub-watershed, $X_{i,w}$ is the decision variable for point source control in each sub-watershed, $Y_{j,w}$ is the decision variable for non-point source control in each sub-watershed, $Z_{k,w}$ is the decision variable for unknown or undetermined source control in each sub-watershed, $C(X_{i,w})$ is the cost of point source control decision variable in a sub-watershed, $C(Y_{j,w})$ is the cost of non-point source control decision variable in a sub-watershed, and $C(Z_{k,w})$ is the cost of unknown or undetermined source control decision variable in a sub-watershed.

For the Beargrass Creek watershed, i and j are equal to 1 (i.e. there is one decision variable for each of the three sub-watersheds that consists of a point source volume control, and one decision variable for each of the three sub-watersheds that consists of a non-point source volume control). In the case of the unknown or undetermined source, the value of n (the index for the unknown source decision variable) varies for the three sub-watersheds. For the South fork sub-watershed, the value of n is four, whereas for the Middle and Muddy fork sub-watersheds, the value of n is three. All the 16 decision variables ($X_{i,w}$, $Y_{j,w}$, and $Z_{k,w}$) in the optimal management model are defined in Figure 7-7.

South Fork Decision Variables	Middle Fork Decision Variables	Muddy Fork Decision Variables
$X_{1,1}$ = Point Source Volume	$X_{1,2}$ = Point Source Volume	$X_{1,3}$ = Point Source Volume
$Y_{1,1}$ = Non-point Source Volume	$Y_{1,2}$ = Non-point Source Volume	$Y_{1,3}$ = Non-point Source Volume
$Z_{1,1}$ = Leaking Sewer Length (class 1)	$Z_{1,2}$ = Leaking Sewer Length (class 1)	$Z_{1,3}$ = Leaking Sewer Length (class 1)
$Z_{2,1}$ = Leaking Sewer Length (class 2)	$Z_{2,2}$ = Leaking Sewer Length (class 2)	$Z_{2,3}$ = Leaking Sewer Length (class 2)
$Z_{3,1}$ = Leaking Sewer Length (class 3)	$Z_{3,2}$ = Leaking Sewer Length (class 3)	$Z_{3,3}$ = Leaking Sewer Length (class 3)
$Z_{4,1}$ = Leaking Sewer Length (class 4)		

Figure 7-7. Decision variables in the optimal management formulation

7.4.2 Constraints

The objective function as described in Equation (7-1) above is subject to three types of constraints: 1) a set of implicit system constraints, 2) a set of implicit bound constraints, and 3) a set of explicit decision variable bound constraints.

7.4.2.1 Implicit System Constraints

The evaluation of dissolved oxygen for each of the three sub-watersheds requires a simulation model that relates the dissolved oxygen to the organic load (BOD concentration in mg/L and associated flows). The inverse loading BOD model developed for the Beargrass Creek watershed was used to represent the implicit system constraints in the optimal management model. This simple deductive model is based on the classic Streeter-Phelps (Streeter and Phelps, 1925) dissolved oxygen deficit equation. The decision variables (as given in Figure 7-7) from the optimization model ($X_{i,w}$, $Y_{j,w}$, and $Z_{k,w}$) will be passed on to this simulation model which will in turn compute the effective BOD load for each of the three sub-watersheds corresponding to a particular management strategy. The inverse-loading BOD model is described as follows.

<u>Streeter-Phelps Dissolved Oxygen Model</u>

A simple, conceptual, and macro-level dissolved oxygen model was developed for each of the three forks of Beargrass Creek watershed using the classic Streeter-Phelps equations (Streeter and Phelps, 1925). The dissolved oxygen in a stream, DO, depends on the oxygen deficit D and the saturation dissolved oxygen DO_{sat} as given by Equation 7-2. The oxygen deficit is a function of the initial deficit Do, effective BOD concentration L_o, BOD decay rate K_d, and re-aeration from the atmosphere K_a, and is given by Equation 7-3. Figure 7-8 gives a sketch of the DO dynamics along the length of a given stream segment.

$$DO = DO_{sat} - D \tag{7-2}$$

$$D = D_o\, e^{\left(\frac{-Ka}{U}\right)X} + \frac{K_d\, L_o}{K_a - K_d}\left(e^{\left(\frac{-Kd}{U}\right)X} - e^{\left(\frac{-Ka}{U}\right)X}\right) \tag{7-3}$$

Where	Do	=	initial deficit
	L_o	=	ultimate BOD concentration (mg/L)
	K_a	=	re-aeration rate (day)-1

K_d	=	decay rate (day)-1
U	=	average velocity in the stream (feet per day)
X	=	length of the stream (feet)

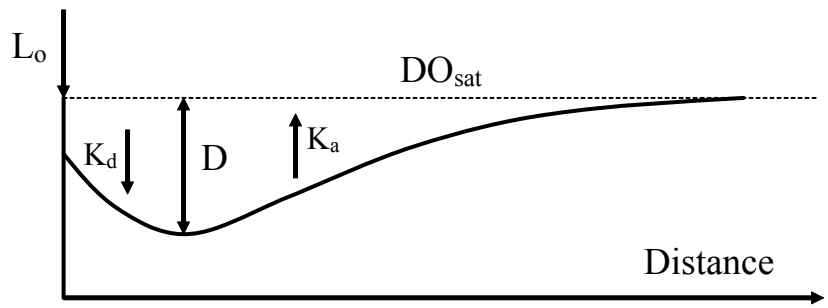


Figure 7-8. Dissolved oxygen deficit in a stream

For the Beargrass Creek watershed, there are three stream segments in the model corresponding to the three sub-watersheds. A schematic of the stream segments in each of the three sub-watersheds is given in Figure 7-9 below.

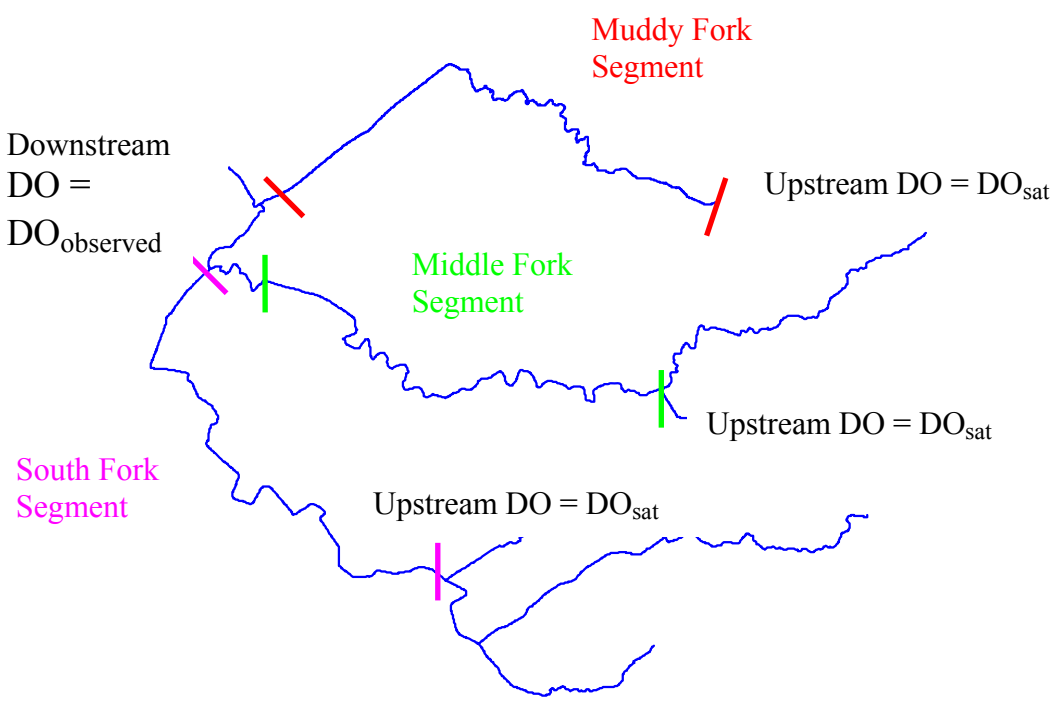


Figure 7-9. Schematic of the Simplified Deductive DO Model for three Forks of the Beargrass Creek Watershed

Solving Equation (7-3) for L_o and assuming initial deficit to be zero yields Equation (7-4) as given below.

$$L_o = \frac{(K_a - K_d)D}{\left(e^{\left(\frac{-Kd}{U}\right)X} - e^{\left(\frac{-Ka}{U}\right)X} \right)} \qquad (7\text{-}4)$$

A daily time step was used in the steady state dissolved oxygen model. Based on the actual average daily DO deficit observed between the most upstream and downstream stations of each of the three stream, Equation (7-4) was used to back-calculate the effective BOD concentration for each stream that is causing the observed deficit. Initial deficit is assumed to be zero as the DO in the most upstream end of the each of the streams is fairly close to the saturation DO. The rate of decay (K_d) is assumed to be 0.25 (Chapra, 1997) (suggested range of 0.15 to 0.35 in most text books). The re-aeration rate (K_a) is computed based on the average velocity and depth in the stream by using Equation 7-5 (O'Connor and Dobbins, 1958), Equation 7-6 (Churchill et al. 1962), or Equation 7-7 (Owens, et al. 1964). The depth and velocity terms used in Equations 7-5 through 7-7 were computed by using relationships derived from actual rating curves developed for all of the USGS gauging stations of the watershed.

$$K_a = 12.9\left(\frac{Velocity^{0.5}}{Depth^{1.5}}\right) \qquad (7\text{-}5)$$

$$K_a = 11.6\left(\frac{Velocity}{Depth^{1.67}}\right) \qquad (7\text{-}6)$$

$$K_a = 21.6\left(\frac{Velocity^{0.67}}{Depth^{1.85}}\right) \qquad (7\text{-}7)$$

The total average daily flow is obtained for each of the three forks by utilizing the data collected at five USGS gauging stations in the watershed. Average daily flow is

segregated into three components corresponding to the three sources namely (as shown in schematically in Figure 7-10):

4. Point source flow from CSO discharges,
5. Non-point source flow from urban runoff, and
6. Base flow in the stream.

The contribution of CSO flows for a particular stream reach is approximated by using USGS gauging stations upstream and downstream of the CSO areas as follows. First, the total contributing drainage area between the two USGA stations was determined and separated into a CSO drainage area and a non-CSO drainage area using the GIS database for the watershed. This will establish the percentage of CSO drainage area for a particular stream reach between the two USGS gauging stations. Second, the difference of stream flow is computed between the two USGS gauging stations on a particular stream reach. Lastly, the percentage of CSO areas computed in the first step is applied to the difference flow computed in the second step to get an approximation of the CSO component of the stream flow for a particular stream reach. The remaining flow is assumed to be contributed by storm water runoff due to the non-CSO drainage area in the stream reach. In addition, a constant base flow is assumed based on the actual total flow hydrograph obtained at the USGS sites.

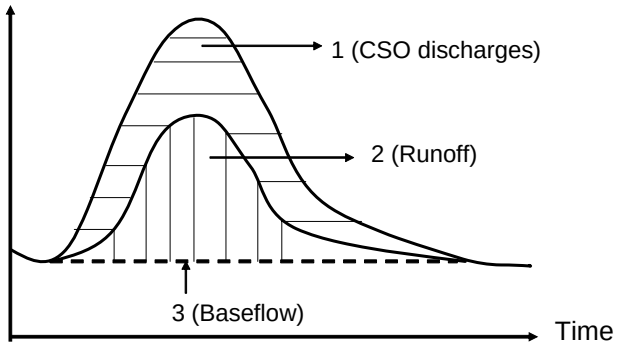


Figure 7-10. Segregation of daily average flows for each fork of Beargrass Creek

Once the effective daily ultimate BOD concentration (L_o) is computed for each of the three streams, a mass balance of flow and concentration for each of the contributing sources is performed to quantify the BOD concentration from each source. Three types of sources are identified to be contributing BOD loads into the stream segments including:

1. Point source contribution of BOD loads from CSO events during storm event.
2. Non-point source contribution of BOD loads from storm water runoff.
3. An unknown or undetermined source of BOD contribution that is associated with the base flow in the streams. Such an unknown source may include other suspected sources of BOD contribution such as sediment oxygen demand (SOD) or ex-filtration from leaking sewers (that run close to the stream segments in the model) onto the stream banks.

The total BOD concentration (calculated from Equation 7-4) can be represented as a mass balance of the flow and concentration from the three sources of flow and BOD concentration identified above and is given by Equation 7-8 below:

$$L_o\ (Total\ BOD) = \left(\frac{Q_{PS} * L_{PS} + Q_{NPS} * L_{NPS} + Q_{BF} * L_{UKS}}{Q_{PS} + Q_{NPS} + Q_{BF}} \right) \tag{7-8}$$

Where	L_o	=	Total ultimate BOD concentration in mg/L
	Q_{PS}	=	point source flow (CSO discharges) in ft3/sec
	Q_{NPS}	=	non-point source flow (urban runoff) in ft3/sec
	Q_{BF}	=	base flow in ft3/sec
	L_{PS}	=	BOD concentration of CSO discharges in mg/L
	L_{NPS}	=	BOD concentration of urban runoff in mg/L
	L_{UKS}	=	BOD concentration of the unknown source

BOD concentration values were assigned to the point and non-point source contributions based on a survey of literature values (Tetra Tech, 2005) and used in Equation 7-9 to obtain the BOD concentration for the unknown source. Literature values used for L_{PS} = 50 mg/L and L_{NPS} = 10 mg/L. These can obviously be changed if actual values are available either from sampling or as an output from a more detailed process-based model of the watershed.

$$L_{UKS} = \frac{\left(L_o * \left(Q_{PS} + Q_{NPS} + Q_{BF}\right) - \left(Q_{PS} * L_{PS}\right) - \left(Q_{NPS} * L_{NPS}\right)\right)}{Q_{BF}} \tag{7-9}$$

Once the unknown source BOD concentration is determined, the model is used in the forward direction to compute DO at the downstream end of each of the three forks of the Beargrass Creek. The DO simulation model as described above is used to obtain the time series of DO for the three sub-watersheds and the two confluence locations (confluence of South and Middle Forks and the confluence of South and Muddy Forks) for the period October 1, 2003 to September 30, 2004. After initial screening of the data and discarding any suspicious observations, the resulting time series of DO consists of a total of 267 days. A mass balance of DO and stream flow is performed to compute the DO at the confluence of the forks.

In the context of the optimization, each time a management strategy is evaluated, the decision variables are passed to the simulation model. Each set of decision variables constituting a management strategy has an affect on the total BOD concentration L_o (as given in Equation 7-8) for a given time step in a given sub-watershed. This effect on L_o is translated into a corresponding effect on the DO time series computed for each of the three sub-watersheds when the simulation models is run in the forward direction using Equation (7-3). This is achieved in the following manner:

1. Effect of point source-related decision variables

   Each set of decision variables consists of a point source volume ($X_{i,w}$) for all three sub-watersheds. When passed to the simulation model, this volume is compared against the actual point source flow for the given time step and sub-watershed. If the value of the point source volume decision variable is equal or greater than the actual point source flow, the point source flow (Q_{PS}) in Equation (7-8) is set to zero. This means that all of the point source flow (resulting from a CSO event) is being stored per the management strategy evaluated. Alternatively, if the value of the point source volume decision variable is less than the actual point source flow, the point source flow (Q_{PS}) is set to the difference between the point source volume decision variable and the actual point source flow (expressed as a daily volume). This means that a portion of the point source flow (Q_{PS}) is being stored per the management strategy, and the remaining will be used in the forward DO simulation model to compute the time series of DO using Equation (7-3). Point source related decision variables ($X_{i,w}$) in a given strategy will thus have an impact on the effective BOD concentration (L_o) computed using Equation (7-8). Consequently, by changing the effective BOD load (L_o), a corresponding change is observed in DO time series for each sub-watershed computed using Equation (7-3) for the particular management strategy evaluated. This is mathematically stated as follows:

$$Q_{PS}(new) = \left\{ \begin{array}{ll} 0, & if \left(\frac{X_{i,w}}{t}\right) \geq Q_{PS} \\ \left(\frac{X_{i,w}}{t}\right) - Q_{PS}, & if \left(\frac{X_{i,w}}{t}\right) < Q_{PS} \end{array} \right\} \quad (7\text{-}10)$$

   Where $Q_{PS}(new)$ is the modified point source flow reflecting the effect of the point source related decision variables, Q_{PS} is the actual point source contribution in the total stream flow time series (resulting from a CSO event), X_{iw} is the point source volume decision variable passed from the optimization model to the simulation model, and t is the daily time step used in the model.

2. Effect of non-point source-related decision variables

Each set of decision variables consists of a non-point source volume ($Y_{j,w}$) for all three sub-watersheds. This represents a detention/retention basin for the sub-watershed that can be used to treat the storm water runoff and reduce or eliminate the BOD concentration in storm water runoff. When passed to the simulation model, this volume is compared against the actual non-point source flow (runoff component of the hydrograph) for the given time step and sub-watershed. This non-point source volume decision variable has an effect on the BOD concentration of non-point source flow component (L_{NPS}) as given in Equation (7-8). Depending on the volume of storage provided by the management strategy for storing non-point source flow (i.e. the value of $Y_{j,w}$), either all or portion of the actual non-point source flows component is treated for BOD reduction. If the value of ($Y_{j,w}$) is greater or equal to the actual non-point source flow for a sub-watershed, all of the flow is treated for BOD removal. Alternatively, if the value of ($Y_{j,w}$) is less than the actual non-point source flow for a sub-watershed, the difference is treated for BOD removal. It is assumed that any portion of the non-point source flow stored will result in a 90% removal of BOD concentration in the non-point source flow. Thus for a particular management strategy and corresponding non-point source decision variable, the simulation model will compute a modified BOD load resulting from the non-point source component. The modified non-point source BOD load (flow multiplied by concentration) resulting from a particular management strategy is mathematically given as follows:

$$BOD\,Load_{NPS}(new) = (Q_{NPS}(treated) * (L_{NPS} * 0.1)) + (Q_{NPS}(untreated) * L_{NPS}) \quad (7\text{-}11)$$

Where $BOD\,Load_{NPS}$ (new) represents the modified BOD load for use in Equation (7-8) to compute the total effective BOD concentration (L_o) reflecting the effect of the non-point source related decision variables ($Y_{j,w}$) and L_{NPS} is the non-point source BOD concentration. Consequently, by changing the effective BOD load (L_o), a

corresponding change is observed in DO time series for each sub-watershed computed using Equation (7-3) for the particular management strategy evaluated.

3. Effect of unknown source-related decision variables

   Each set of decision variables consists of multiple unknown sources related decision variables ($Z_{k,w}$) for all three sub-watersheds. Each of these represents a length of leaking sewers in the proximity of the streams that need to be lined to eliminate ex-filtration of BOD concentration onto the stream banks. When passed to the simulation model, the length in each of these decision variables is compared against the actual length of sewers in each sub-watershed. If the length of sewer in a particular management strategy for a particular sub-watershed is equal to the actual length of the sewer, all of the sewers in that sub-watershed are lined or rehabilitated. This means that the BOD concentration corresponding to the unknown source (represented by L_{UKS} in Equation 7-8) for that sub-watershed is eliminated. If the length of sewer in a particular management strategy for a particular sub-watershed is less than the actual length of the sewer, a percentage of sewers are lined per the management strategy. The corresponding decrease in the unknown source related BOD concentration is proportional to the percentage of sewers that are being lined per the management strategy. Thus each set of decision variables related to the unknown source in each sub-watershed results in reduction of the corresponding BOD concentration (L_{UKS}). This will in effect change the total effective BOD concentration as computed by Equation (7-8). Unknown source related decision variables ($Z_{k,w}$) in a given strategy will thus have an impact on the effective BOD concentration (L_o) computed using Equation (7-8). Consequently, by changing the effective BOD load (L_o), a corresponding change is observed in DO time series for each sub-watershed computed using Equation (7-3) for the particular management strategy evaluated

7.4.2.2 Implicit Bound Constraints

The implicit bound constraints include the constraints on the dissolved oxygen in each of the three forks to be equal to or greater than a prescribed threshold level as required by the State of Kentucky regulations for aquatic life. Per Kentucky Water Quality Standards, the dissolved oxygen criterion for aquatic life is 5.0 mg/L (daily average) and 4.0 mg/L (instantaneous minimum) (Kentucky Administrative Regulations Title 401, Chapter 5, Water Quality). For each day of the DO simulation model, the dissolved oxygen must be greater than such a prescribed standard value. This may be expressed as follows:

$$DO(X_i, Y_j Z_k) \quad \geq \quad WQ_{standard} \qquad \forall\, w, t \qquad (7\text{-}12)$$

Where *w* refers to a sub-watershed and *t* refers to the time step in the simulation model. Thus for each set of decision variables in a management strategy, the model computed dissolved oxygen should be greater than or equal to the prescribed standard. If the DO does not meet the standard, a violation is recorded by the model. For the proposed optimal management model for Beargrass Creek watershed, three different standards were used in the model to evaluate the performance of the model under different DO standards. These included average daily standards of 4.0 mg/L, 5.0 mg/L, and 6.0 mg/L.

7.4.2.3 Explicit Decision Variable Bound Constraints

The final set of bound constraints consists of explicit bounds on the decision variables. In this case, each of the 16 decision variables given in Figure 7-7 (six for South fork, five for Middle fork, and five for Muddy fork) will be restricted between a lower value of zero (corresponding to a no improvement strategy) and an upper value (corresponding to the maximum possible rehabilitation strategy). Mathematically, this may be expressed as given in Equations 7-13 through 7-15 as follows:

$$0 \quad \leq \quad X_{iw} \quad \leq \quad X_{\max} \qquad \forall\, i, w \qquad (7\text{-}13)$$

$$0 \quad \leq \quad X_{jw} \quad \leq \quad X_{\max} \qquad \forall\, j, w \qquad (7\text{-}14)$$

$$0 \leq X_{kw} \leq X_{\max} \qquad \forall\, k, w \qquad (7\text{-}15)$$

Where w refers to a sub-watershed and i, j, and k refers to the three types of pollution sources. The explicit bounds on the decision variables of the optimal management model were established for each of the three sub-watersheds and corresponding pollution source variables. For point source related decision variables, the lower bound is set to zero (no storage required in the management strategy), while the upper bound is set at the maximum volume required for storage during a CSO event. The upper bound was obtained from the time series of flows that are segregated into point sources (CSO flows), non-point sources (runoff), and base flow. Likewise, the lower bound of the non-point source related decision variables are set tot zero (no storage required in the management strategy), and the upper bound is set to the maximum storage required for control of runoff. For the decision variables in the rehabilitation strategy of leaking sewers, the lower bound is set to zero (no sewer lining in the watershed) and the upper bound is set to the maximum length of a particular class of sewer in each watershed. These bounds on the decision variables for each sub-watershed are summarized in Table 7-2.

Table 7-2. Explicit Bounds on Decision Variables in Management Model

Decision Variable	Lower Bound	Upper Bound
$X_{1,1}$	0	202 MG
$X_{1,2}$	0	390 MG
$X_{1,3}$	0	80 MG
$Y_{1,1}$	0	401 MG
$Y_{1,2}$	0	390 MG
$Y_{1,3}$	0	158 MG
$Z_{1,1}$	0	20,200 feet
$Z_{2,1}$	0	26,700 feet
$Z_{3,1}$	0	17,000 feet
$Z_{4,1}$	0	2,300 feet
$Z_{1,2}$	0	13,200 feet
$Z_{2,2}$	0	27,300 feet
$Z_{3,2}$	0	15,900 feet
$Z_{1,3}$	0	19,800 feet
$Z_{2,3}$	0	39,100 feet
$Z_{3,3}$	0	3,900 feet

7.4.3 Cost Data for the Optimal Management Model

The cost of the management strategies used in the management model was derived using EPA recommendations and construction estimates of municipal infrastructure works. These are described as follows (EPA, 2002).

Cost of Volume Controls for Point Sources

Deep tunnel storage option is used for storing the CSO discharges during a storm event. EPA (2002) costs curves for providing this type of storage in a watershed were used in the optimal management model to compute the cost of point source management strategies. For deep tunnel storage, this is given as follows:

$$C = 7.785\ V^{0.795} \qquad (7\text{-}16)$$

Where C = construction cost in 1999 Million $

V = volume of storage system in Million Gallons

The above relationship was updated to December 2005 dollars in the optimal management model.

Cost of Volume Controls for Non-Point Sources

Retention and/or detention basins are commonly used to control urban runoff during a storm event and this storage option was used for storing the urban runoff during a storm event in the optimal management model. EPA (2002) costs curves for providing this type of storage in a watershed were used to compute the cost of non-point source management strategies. For detention basins, this is given as follows.

$$C = 61{,}000\ V^{0.75} \qquad (7\text{-}17)$$

Where C = construction cost in 1999 $

V = volume of basin in Million Gallons

The above relationship was updated to December 2005 dollars in the optimal management model.

Cost of Rehabilitation Strategy for the Leaking Sewers in the Watershed

A comprehensive rehabilitation strategy was formulated for the leaking sewers in the Beargrass Creek watershed. First, all the major sewers along or in close proximity to the banks of the three forks (South, Middle, and Muddy) of the watershed were identified. For each of the three forks, the sewers identified were assigned to a major class of sewers based on its diameter. Accordingly, four classes of sewers were identified in the South Fork watershed, three classes in the Middle Fork watershed, and three classes in the Muddy Fork watershed. A listing of these classes and their corresponding lengths are given for each of the three sub-watersheds in Tables 7-3 through 7-5.

Table 7-3. Sewers in South Fork Watershed

Class of Sewers	Diameter Range (inches)	Length (feet)
1	8-21	20,200
2	24-42	26,700
3	48-66	17,000
4	84-132	2,300

Table 7-4. Sewers in Middle Fork Watershed

Class of Sewers	Diameter Range (inches)	Length (feet)
1	8-18	13,200
2	24-42	27,300
3	48-60	15,900

Table 7-5. Sewers in Muddy Fork Watershed

Class of Sewers	Diameter Range (inches)	Length (feet)
1	6-21	19,800
2	24-30	39,100
3	36	3,900

A unit cost of lining these sewers was estimated by using actual bidding documents for some representative sewer projects in the state of Kentucky (Davis, 2005). These are given in Table 7-6.

Table 7-6. Sewer Lining Costs

Pipe Diameter (inches)	Unit Cost of Lining ($)
6	35
8	40
10	40
12	50
15	60
18	65
21	75
24	90
27	100
30	110
33	125
36	140
39	160
42	180
45	200
48	220

7.4.4 Solution Methodology

The optimal management model is used to evaluate multiple management strategies comprising of different combinations of the 16 decision variables. The effect of these strategies is evaluated on the watershed response via the macro-level deductive dissolved oxygen (DO) simulation model. The objective of the model is to search for the optimal management strategy that is least-cost and achieves the goal of enhancing the DO in the receiving streams above the prescribed water quality standards. Two different optimization models are used to solve the optimal management problem as formulated above. These include the GA-based optimization model and the Shuffled Box Complex-based optimization models. The solution methodology for solving the optimal management model is described in Chapter 6 and shown schematically in Figure 6-4 (GA-based solution) and Figure 6-5 (Shuffled Box Complex-based solution).

7.4.5 Results of the Water Quality-Based Optimal Management Model

7.4.5.1 Results of the Genetic Algorithm-based Model

The objective of the water quality-based optimal management model is to minimize costs associated with a management strategy that satisfies prescribed water quality constraints. In the Beargrass Creek watershed, the water quality problem in hand is the dissolved oxygen impairment. Figure 7-11 and Table 7-7 gives the number of impairment days in the three contributing sub-watersheds for three different DO standards evaluated in the simulation model. As shown in Figure 7-11 and Table 7-7, Muddy fork sub-watershed is least sensitive to the DO standard enforced in a particular simulation of the model. This sub-watershed also has the most impairment of all sub-watersheds. For the remaining two sub-watersheds, the number of DO impairments slightly increase as the DO standard is made more stringent from 4.0 mg/L to 6.0 mg/L.

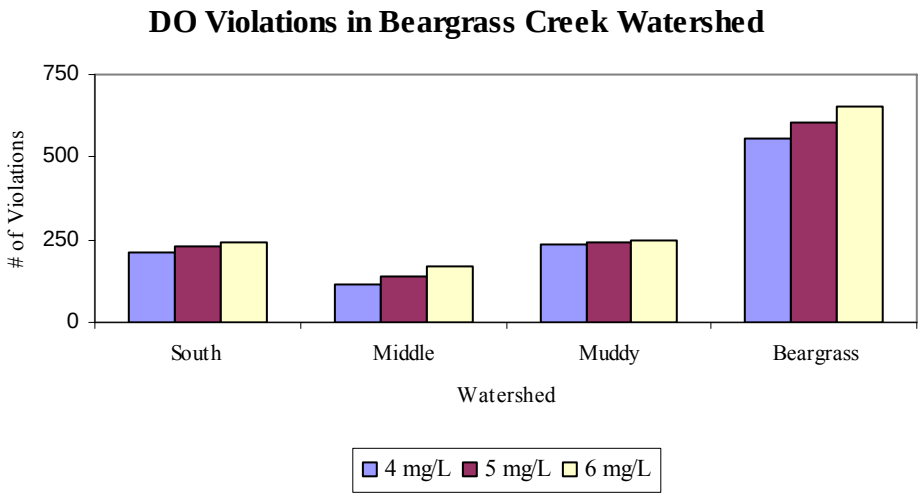


Figure 7-11. DO Violations in the Beargrass Creek Watershed under existing conditions

Table 7-7. DO Violation Days in Beargrass Creek Watershed under Existing Conditions

Watershed	DO Violation for 4 mg/L (Days)	DO Violation for 5 mg/L (Days)	DO Violation for 6 mg/L (Days)
South	210	229	239
Middle	114	138	169
Muddy	234	239	247
Beargrass Creek[1]	558	606	655

(1): The number of violation days for Beargrass Creek is the sum of the violations days in South, Middle, and Muddy Fork sub-watersheds.

The optimal management model was run per the solution methodology described above. The GA-based optimization was performed with different population sizes and varying number of generations. The population size was varied between 30 and 200 whereas the number of generations in the model run was varied from 100 to 1000. In the majority of model runs, the model that utilizes a population of 100 gave optimal results. The model was also analyzed for sensitivity related to the probability of crossover and mutation. The model performed consistently better with a probability of crossover set to 0.7 and the probability of mutation set to 0.03. The results of the optimal management model for the three DO standards (4, 5, and 6 mg/L) enforced are summarized in Figure 7-12 and Tables 7-8 through 7-11.

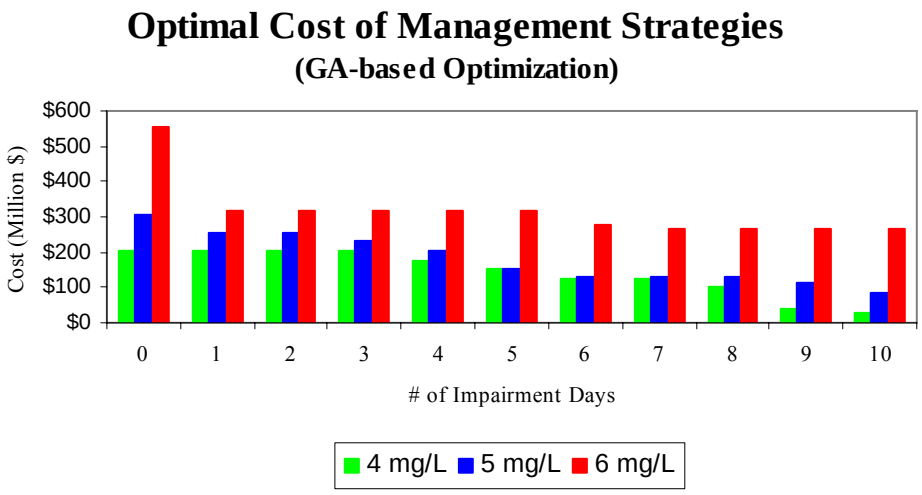


Figure 7-12. Optimal Cost of Management Strategies using GA-based Optimization

Table 7-8. Optimal Management Costs for Beargrass Creek Watershed (Water Quality-based Optimization using GA)

# of Violations	Optimal Cost for 4 mg/L (M$)	Optimal Cost for 5 mg/L (M$)	Optimal Cost for 6 mg/L (M$)
0	203	304	554
1	203	257	319
2	201	257	319
3	201	232	319
4	177	206	319
5	151	151	319
6	123	128	277
7	123	128	268
8	103	128	264
9	41	116	264
10	29	84	264

Table 7-9. Optimal Management Costs for South Fork Sub-Watershed (Water Quality-based Optimization using GA)

# of Violations	South Fork Point Source Costs (M$)	South Fork Non-Point Source Costs (M$)	South Fork Unknown Source Costs (M$)	South Fork Total Costs (M$)	Beargrass Creek Total Costs (M$)	South Fork Costs (% of Total)
0	79.97	0.00	8.85	88.82	203.18	44
0	79.97	6.05	11.07	97.11	303.95	32
0	138.80	2.65	11.00	152.40	554.24	27
1	79.97	0.00	8.85	88.82	203.18	44
1	79.97	6.55	11.06	97.59	257.39	38
1	138.80	6.05	11.95	156.80	318.64	49
2	79.97	0.00	7.51	87.49	201.15	43
2	79.97	6.55	11.06	97.59	257.39	38
2	138.80	6.05	11.95	156.80	318.64	49
3	79.97	0.00	7.51	87.49	201.15	43
3	79.97	6.55	11.43	97.96	231.63	42
3	138.80	6.05	11.95	156.80	318.64	49
4	79.97	0.00	9.61	89.59	177.32	51
4	79.97	5.54	9.97	95.50	205.60	46
4	138.80	6.05	11.95	156.80	318.64	49
5	0.00	1.96	11.31	13.27	150.52	9
5	0.00	1.96	11.31	13.27	150.52	9
5	138.80	6.05	11.95	156.80	318.64	49
6	0.00	5.54	8.08	13.63	122.91	11
6	0.00	3.29	11.61	14.91	128.17	12
6	138.80	8.88	10.70	158.40	276.59	57
7	0.00	5.54	7.91	13.46	122.74	11
7	0.00	3.29	11.61	14.91	128.17	12
7	138.80	3.89	9.81	152.50	268.05	57
8	0.00	8.43	8.23	16.67	102.63	16
8	0.00	3.29	11.61	14.91	128.17	12
8	79.97	2.65	10.54	93.17	264.37	35
9	0.00	7.51	10.51	18.02	41.07	44
9	79.97	1.96	11.80	91.74	116.02	81
9	79.97	2.65	10.54	93.17	264.37	35
10	0.00	0.00	8.58	8.58	28.98	30
10	0.00	8.43	11.39	19.83	83.76	24
10	79.97	2.65	10.54	93.17	264.37	35

Table 7-10. Optimal Management Costs for Middle Fork Sub-Watershed (Water Quality-based Optimization using GA)

# of Violations	Middle Fork Point Source Costs (M$)	Middle Fork Non-Point Source Costs (M$)	Middle Fork Unknown Source Costs (M$)	Middle Fork Total Costs (M$)	Beargrass Creek Total Costs (M$)	Middle Fork Costs (% of Total)
0	0.00	5.93	7.03	12.96	203.18	6
0	0.00	6.89	10.32	17.22	303.95	6
0	138.80	3.81	10.02	152.60	554.24	28
1	0.00	5.93	7.03	12.96	203.18	6
1	0.00	7.81	9.04	16.86	257.39	7
1	0.00	5.42	9.77	15.20	318.64	5
2	0.00	5.93	7.03	12.96	201.15	6
2	0.00	7.81	9.04	16.86	257.39	7
2	0.00	5.42	9.77	15.20	318.64	5
3	0.00	5.93	7.03	12.96	201.15	6
3	0.00	3.81	6.36	10.18	231.63	4
3	0.00	5.42	9.77	15.20	318.64	5
4	0.00	4.37	8.51	12.89	177.32	7
4	0.00	5.93	6.91	12.84	205.60	6
4	0.00	5.42	9.77	15.20	318.64	5
5	0.00	7.35	7.77	15.14	150.52	10
5	0.00	7.35	7.77	15.14	150.52	10
5	0.00	5.42	9.77	15.20	318.64	5
6	0.00	2.60	7.09	9.70	122.91	8
6	0.00	4.91	8.53	13.45	128.17	10
6	0.00	8.69	7.60	16.31	276.59	6
7	0.00	2.60	7.09	9.70	122.74	8
7	0.00	4.91	8.53	13.45	128.17	10
7	0.00	5.93	9.12	15.05	268.05	6
8	0.00	3.81	6.74	10.56	102.63	1
8	0.00	4.91	8.53	13.45	128.17	10
8	79.97	6.89	8.67	95.55	264.37	36
9	0.00	7.35	7.33	14.70	41.07	36
9	0.00	5.42	8.87	14.30	116.02	12
9	79.97	6.89	8.67	95.55	264.37	36
10	0.00	1.91	8.81	10.73	28.98	37
10	0.00	7.35	8.92	16.28	83.76	19
10	79.97	6.89	8.67	95.55	264.37	36

Table 7-11. Optimal Management Costs for Muddy Fork Sub-Watershed (Water Quality-based Optimization using GA)

# of Violations	Muddy Fork Point Source Costs (M$)	Muddy Fork Non-Point Source Costs (M$)	Muddy Fork Unknown Source Costs (M$)	Muddy Fork Total Costs (M$)	Beargrass Creek Total Costs (M$)	Muddy Fork Costs (% of Total)
0	91.72	4.41	5.25	101.40	203.18	50
0	179.90	3.50	6.23	189.60	303.95	62
0	238.90	4.41	5.92	249.20	554.24	45
1	91.72	4.41	5.25	101.40	203.18	50
1	137.70	0.57	4.68	142.90	257.39	56
1	137.70	3.50	5.49	146.70	318.64	46
2	91.72	3.73	5.24	100.70	201.15	50
2	137.70	0.57	4.68	142.90	257.39	56
2	137.70	3.50	5.49	146.70	318.64	46
3	91.72	3.73	5.24	100.70	201.15	50
3	115.30	1.93	6.25	123.50	231.63	53
3	137.70	3.50	5.49	146.70	318.64	46
4	66.45	2.22	6.16	74.83	177.32	42
4	91.72	1.32	4.21	97.26	205.60	47
4	137.70	3.50	5.49	146.70	318.64	46
5	115.30	0.57	6.23	122.10	150.52	81
5	115.30	0.57	6.23	122.10	150.52	81
5	137.70	3.50	5.49	146.70	318.64	46
6	91.72	4.19	3.66	99.58	122.91	81
6	91.72	3.25	4.82	99.81	128.17	78
6	91.72	3.73	6.47	101.90	276.59	37
7	91.72	4.19	3.66	99.58	122.74	81
7	91.72	3.25	4.82	99.81	128.17	78
7	91.72	3.01	5.78	100.50	268.05	37
8	66.45	4.19	4.75	75.39	102.63	73
8	91.72	3.25	4.82	99.81	128.17	78
8	66.45	3.01	6.18	75.65	264.37	29
9	0.00	3.01	5.34	8.35	41.07	20
9	0.00	2.75	5.21	7.97	116.02	7
9	66.45	3.01	6.18	75.65	264.37	29
10	0.00	3.73	5.92	9.66	28.98	33
10	38.30	4.41	4.94	47.66	83.76	57
10	66.45	3.01	6.18	75.65	264.37	29

Figures 7-13 and 7-14 provide an analysis of the allocation of total costs by sub-watershed and by pollution types respectively for a specified number of violations allowed in the DO simulation. Figure 7-15 provides the allocation of the number of total violation days allowed between the three sub-watersheds. Figure 7-16 through 7-18 provides the allocation of total costs in each sub-watershed by pollution type for a specified number of violations allowed in the DO simulation. The results given in Figures 7-13 through 7-18 corresponds to a DO standard of 5 mg/L.

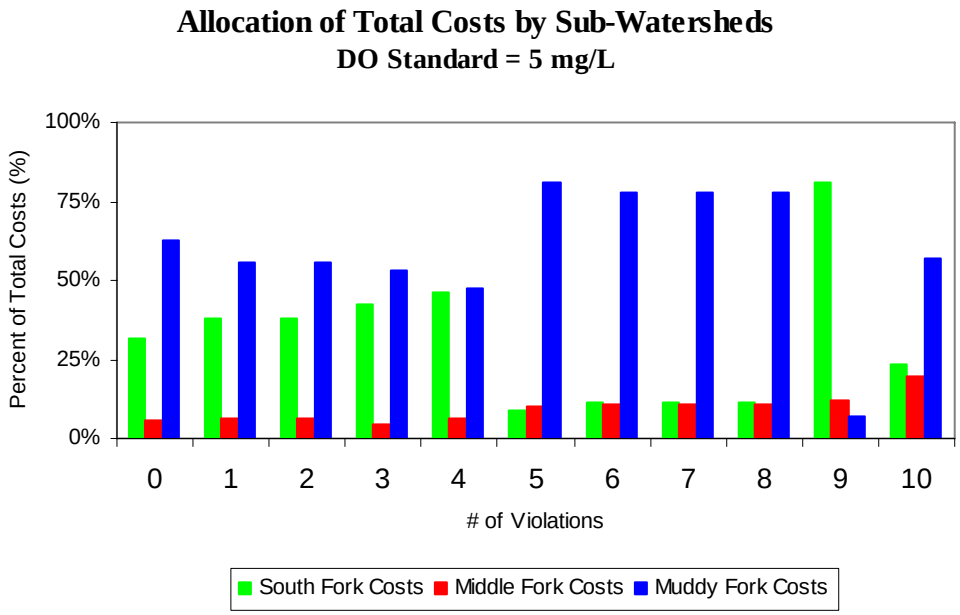


Figure 7-13. Allocation of Total Costs by Sub-watershed in the GA-based Model

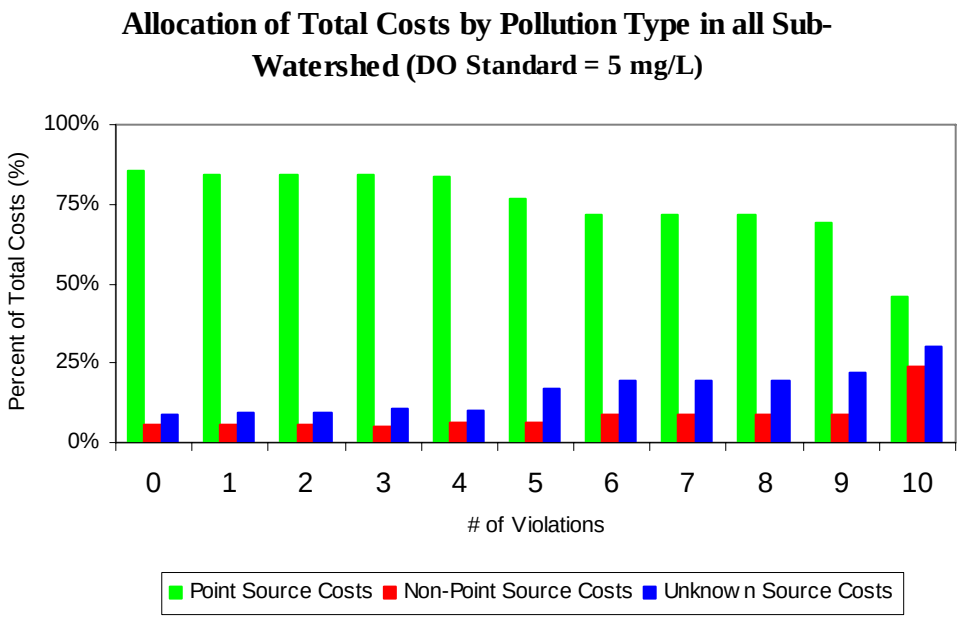


Figure 7-14. Allocation of Total Costs by Pollution Type in the GA-based Model

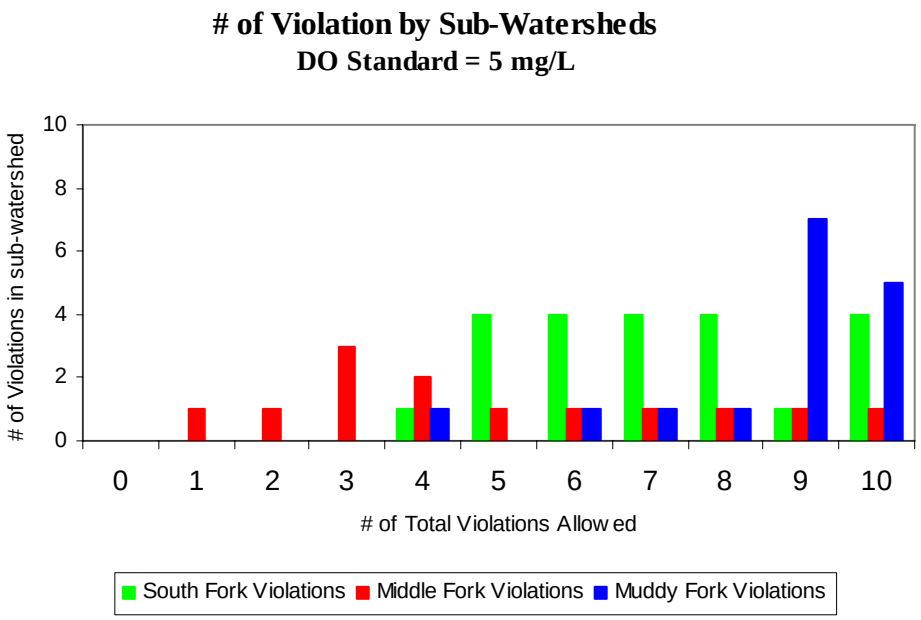


Figure 7-15. Allocation of Total Violation Days in the GA-based Model

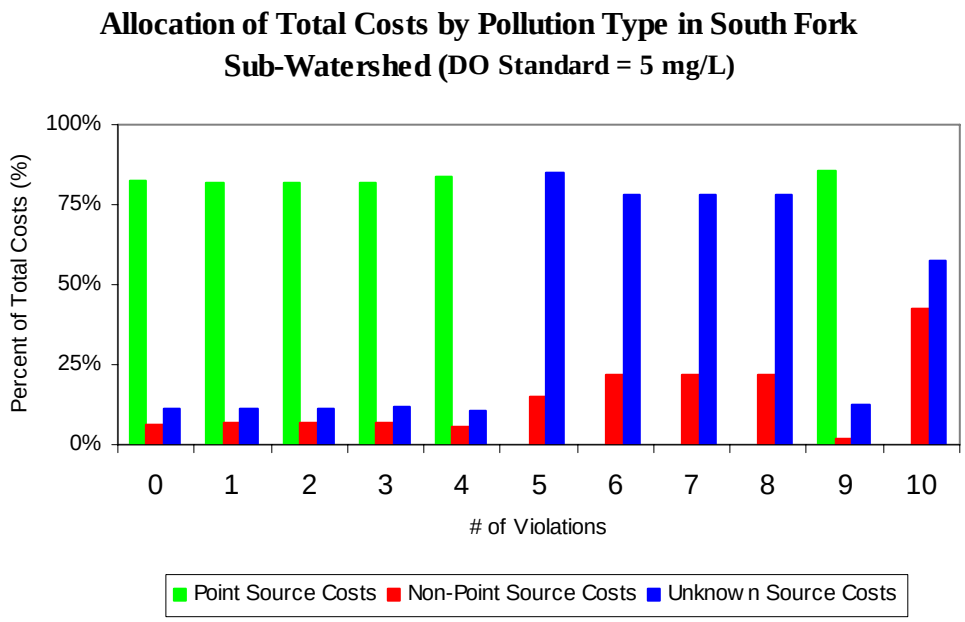


Figure 7-16. Allocation of Total Cost in South Fork by Pollution Type in the GA-based Model

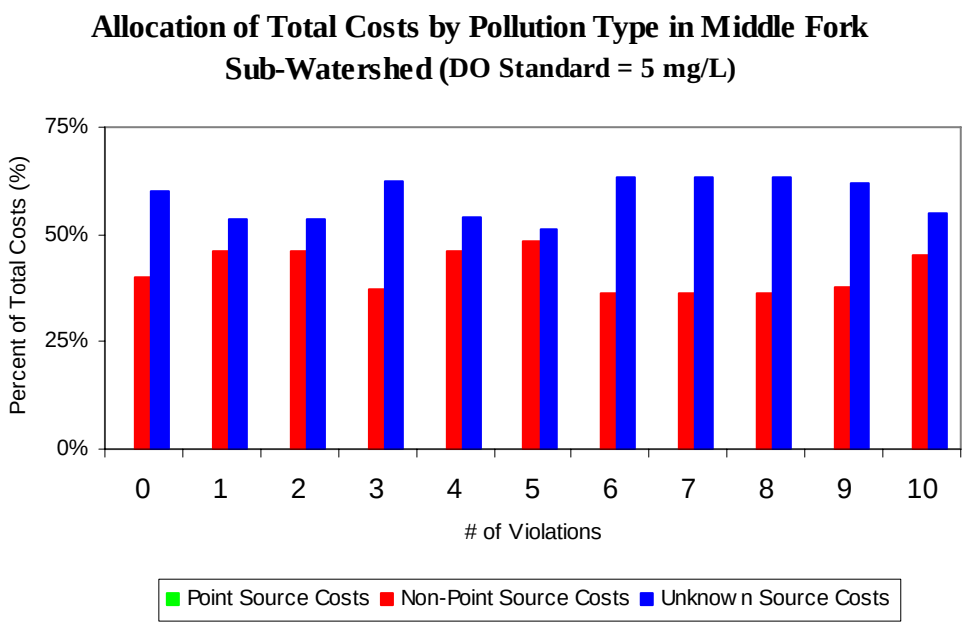


Figure 7-17. Allocation of Total Cost in Middle Fork by Pollution Type in the GA-based Model

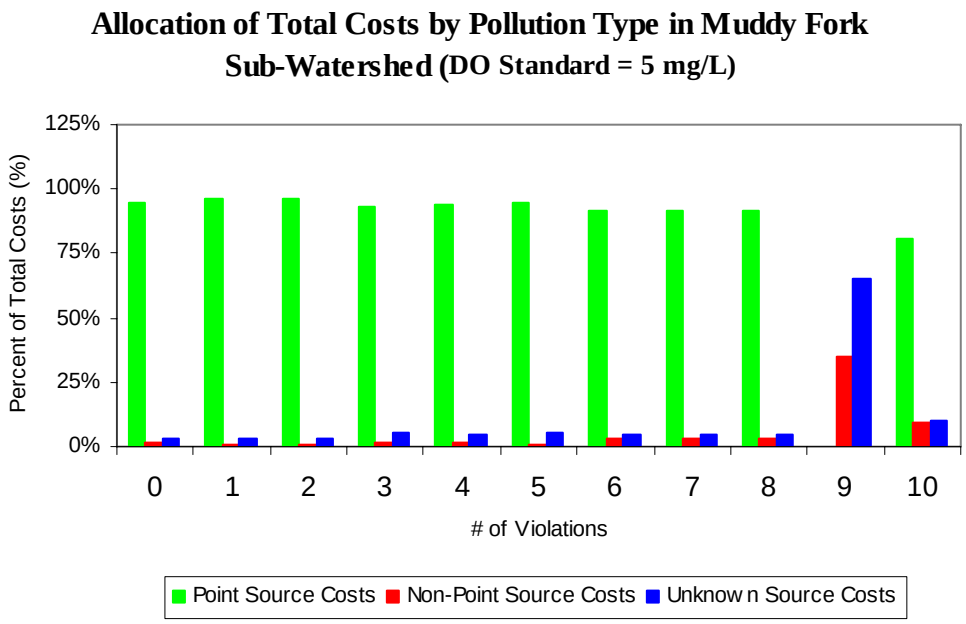


Figure 7-18. Allocation of Total Cost in Muddy Fork by Pollution Type in the GA-based Model

7.4.5.2 Results of the Shuffled Box Complex-based Model

The optimal management model for the Beargrass Creek watershed was run per the solution methodology for the Shuffled Box Complex-based optimization model. Similar to the GA-based management model, this management model also utilizes the inverse-loading macro-level model for simulating the DO response in the watershed. In the Shuffled Box Complex-based optimization, a total of 100 initial feasible solutions sets are sequentially generated to form the complexes in the optimization model. These were partitioned into 5 different complexes, each complex consisting of 20 solution sets (vertices of the complex). The shuffling of the solution sets in each complex was performed after 100, 200, 300, 400, and 500 generations (iterations of the model). The model was run for a total of 1000 generations (iterations). Separate models were evaluated for each of the three DO standards (4, 5, and 6 mg/L). For each DO standard, the model was run for individual constraints (DO impairment days) ranging from 0 to 10 impairment days. The results of the Shuffled-Box Complex-based optimal management

model for the Beargrass Creek watershed for the three DO standards (4, 5, and 6 mg/L) are summarized in Figure 7-19 and Tables 7-12 through 7-15.

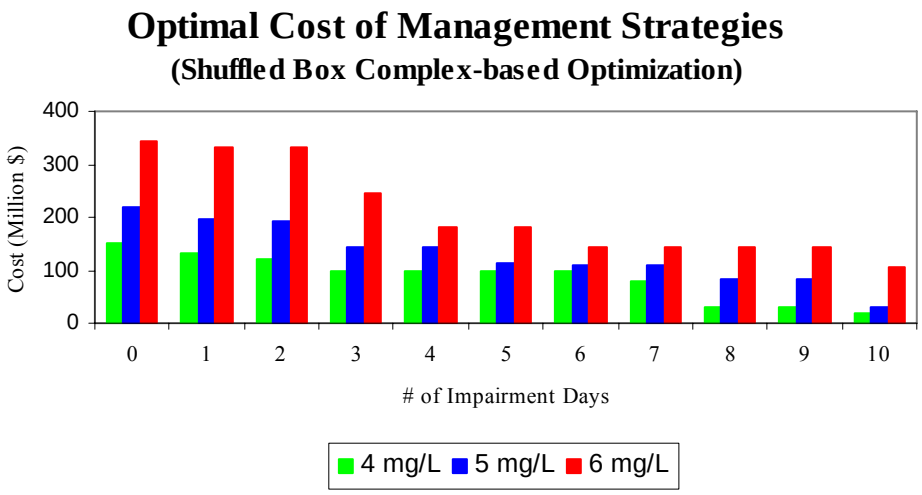


Figure 7-19. Optimal Cost of Management Strategies using Shuffled Box Complex-based Optimization

Table 7-12. Optimal Management Costs for Beargrass Creek Watershed (Water Quality-based Optimization using Shuffled Box Complex)

# of Violations	Optimal Cost for 4 mg/L (M$)	Optimal Cost for 5 mg/L (M$)	Optimal Cost for 6 mg/L (M$)
0	150	220	343
1	131	198	332
2	121	191	332
3	99	144	246
4	99	144	181
5	99	113	181
6	100	111	145
7	79	111	145
8	32	83	145
9	32	83	145
10	21	30	106

Table 7-13. Optimal Management Costs for South Fork Sub-Watershed (Water Quality-based Optimization using Shuffled Box Complex)

# of Violations	South Fork Point Source Costs (M$)	South Fork Non-Point Source Costs (M$)	South Fork Unknown Source Costs (M$)	South Fork Total Costs (M$)	Beargrass Creek Total Costs (M$)	South Fork Costs (% of Total)
0	48.04	0.09	11.94	60.07	149.40	40
0	55.85	8.05	12.15	76.05	219.50	35
0	137.40	8.88	11.51	157.80	342.90	46
1	17.54	2.81	13.00	33.35	130.50	26
1	61.07	0.09	10.10	71.26	197.10	36
1	125.00	1.23	11.27	137.50	331.20	42
2	20.31	0.24	12.21	32.75	121.00	27
2	66.82	8.88	11.43	87.13	191.00	46
2	125.00	1.23	11.27	137.50	331.20	42
3	0.00	0.69	9.41	10.10	98.28	10
3	54.98	3.72	12.54	71.24	144.00	49
3	76.03	8.87	12.23	97.12	245.10	40
4	0.00	0.69	9.41	10.10	98.28	10
4	54.98	3.72	12.54	71.24	144.00	49
4	63.45	8.87	12.50	84.83	181.00	47
5	0.00	0.69	9.41	10.10	98.28	10
5	0.00	0.25	12.63	12.88	112.20	11
5	63.45	8.87	12.50	84.83	181.00	47
6	22.68	0.29	11.65	34.62	99.36	35
6	59.36	0.00	12.53	71.88	110.70	65
6	57.21	0.34	11.62	69.17	145.00	48
7	0.95	0.00	11.02	11.97	78.95	15
7	59.36	0.00	12.53	71.88	110.70	65
7	57.21	0.34	11.62	69.17	145.00	48
8	0.00	8.88	8.52	17.40	31.66	55
8	42.16	0.20	12.96	55.32	82.14	67
8	57.21	0.34	11.62	69.17	145.00	48
9	0.00	8.88	8.52	17.40	31.66	55
9	42.16	0.20	12.96	55.32	82.14	67
9	57.21	0.34	11.62	69.17	145.00	48
10	0.06	0.11	9.21	9.39	20.26	46
10	0.00	0.61	13.00	13.61	29.56	46
10	64.35	0.68	11.79	76.83	105.70	73

Table 7-14. Optimal Management Costs for Middle Fork Sub-Watershed (Water Quality-based Optimization using Shuffled Box Complex)

# of Violations	Middle Fork Point Source Costs (M$)	Middle Fork Non-Point Source Costs (M$)	Middle Fork Unknown Source Costs (M$)	Middle Fork Total Costs (M$)	Beargrass Creek Total Costs (M$)	Middle Fork Costs (% of Total)
0	0.00	0.05	7.29	7.34	149.40	5
0	10.73	8.69	8.68	28.09	219.50	13
0	43.21	7.56	10.68	61.45	342.90	18
1	1.51	2.25	7.11	10.86	130.50	8
1	7.93	8.35	8.87	25.15	197.10	13
1	29.12	8.43	8.37	45.91	331.20	14
2	0.40	0.02	6.23	6.66	121.00	6
2	0.04	0.00	10.16	10.20	191.00	5
2	29.12	8.43	8.37	45.91	331.20	14
3	0.06	0.18	6.06	6.30	98.28	6
3	2.38	0.38	10.40	13.16	144.00	9
3	23.95	8.68	8.40	41.03	245.10	17
4	0.06	0.18	6.06	6.30	98.28	6
4	2.38	0.38	10.40	13.16	144.00	9
4	16.74	8.70	10.49	35.92	181.00	20
5	0.06	0.18	6.06	6.30	98.28	6
5	0.00	0.59	10.36	10.95	112.20	10
5	16.74	8.70	10.49	35.92	181.00	20
6	0.01	5.37	6.74	12.12	99.36	12
6	0.23	0.35	8.93	9.51	110.70	9
6	0.12	0.52	10.35	10.99	145.00	8
7	0.00	8.70	5.66	14.36	78.95	18
7	0.23	0.35	8.93	9.51	110.70	9
7	0.12	0.52	10.35	10.99	145.00	8
8	0.00	0.49	7.15	7.64	31.66	24
8	0.00	8.02	9.44	17.46	82.14	21
8	0.12	0.52	10.35	10.99	145.00	8
9	0.00	0.49	7.15	7.64	31.66	24
9	0.00	8.02	9.44	17.46	82.14	21
9	0.12	0.52	10.35	10.99	145.00	8
10	0.55	0.08	6.11	6.74	20.26	33
10	0.00	0.00	10.70	10.70	29.56	36
10	0.03	0.45	7.83	8.32	105.70	8

Table 7-15. Optimal Management Costs for Muddy Fork Sub-Watershed (Water Quality-based Optimization using Shuffled Box Complex)

# of Violations	Muddy Fork Point Source Costs (M$)	Muddy Fork Non-Point Source Costs (M$)	Muddy Fork Unknown Source Costs (M$)	Muddy Fork Total Costs (M$)	Beargrass Creek Total Costs (M$)	Muddy Fork Costs (% of Total)
0	75.01	1.06	5.95	82.03	149.40	55
0	108.50	0.99	5.91	115.40	219.50	53
0	112.60	4.42	6.65	123.70	342.90	36
1	76.52	4.42	5.32	86.26	130.50	66
1	93.21	0.95	6.51	100.70	197.10	51
1	141.00	1.51	5.26	147.80	331.20	45
2	76.62	0.51	4.50	81.63	121.00	67
2	88.28	0.61	4.76	93.65	191.00	49
2	141.00	1.51	5.26	147.80	331.20	45
3	75.13	0.93	5.82	81.88	98.28	83
3	51.01	4.18	4.42	59.60	144.00	41
3	96.67	4.41	5.83	106.90	245.10	44
4	75.13	0.93	5.82	81.88	98.28	83
4	51.01	4.18	4.42	59.60	144.00	41
4	53.84	0.16	6.26	60.26	181.00	33
5	75.13	0.93	5.82	81.88	98.28	83
5	83.37	0.29	4.71	88.36	112.20	79
5	53.84	0.16	6.26	60.26	181.00	33
6	44.95	4.42	3.25	52.61	99.36	53
6	20.24	4.33	4.77	29.34	110.70	27
6	56.00	3.86	5.01	64.87	145.00	45
7	42.31	4.42	5.89	52.62	78.95	67
7	20.24	4.33	4.77	29.34	110.70	27
7	56.00	3.86	5.01	64.87	145.00	45
8	0.00	0.00	6.62	6.62	31.66	21
8	0.10	4.40	4.86	9.36	82.14	11
8	56.00	3.86	5.01	64.87	145.00	45
9	0.00	0.00	6.62	6.62	31.66	21
9	0.10	4.40	4.86	9.36	82.14	11
9	56.00	3.86	5.01	64.87	145.00	45
10	0.00	0.46	3.67	4.13	20.26	20
10	0.10	0.43	4.79	5.25	29.56	18
10	13.90	0.58	6.09	20.57	105.70	19

Figures 7-20 and 7-21 provide an analysis of the allocation of total costs by sub-watershed and by pollution types respectively for a specified number of violations allowed in the DO simulation. Figure 7-22 provides the allocation of the number of total violation days allowed between the three sub-watersheds. Figure 7-23 through 7-25 provides the allocation of total costs in each sub-watershed by pollution type for a specified number of violations allowed in the DO simulation. The results given in Figures 7-20 through 7-25 corresponds to a DO standard of 5 mg/L.

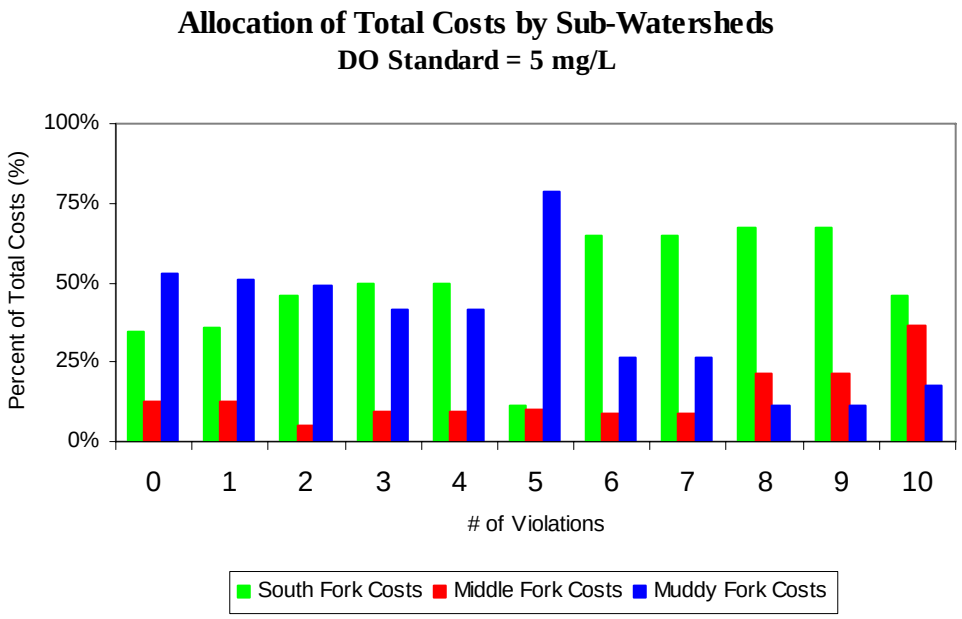


Figure 7-20. Allocation of Total Costs by Sub-watershed in the Shuffled Box Complex-based Model

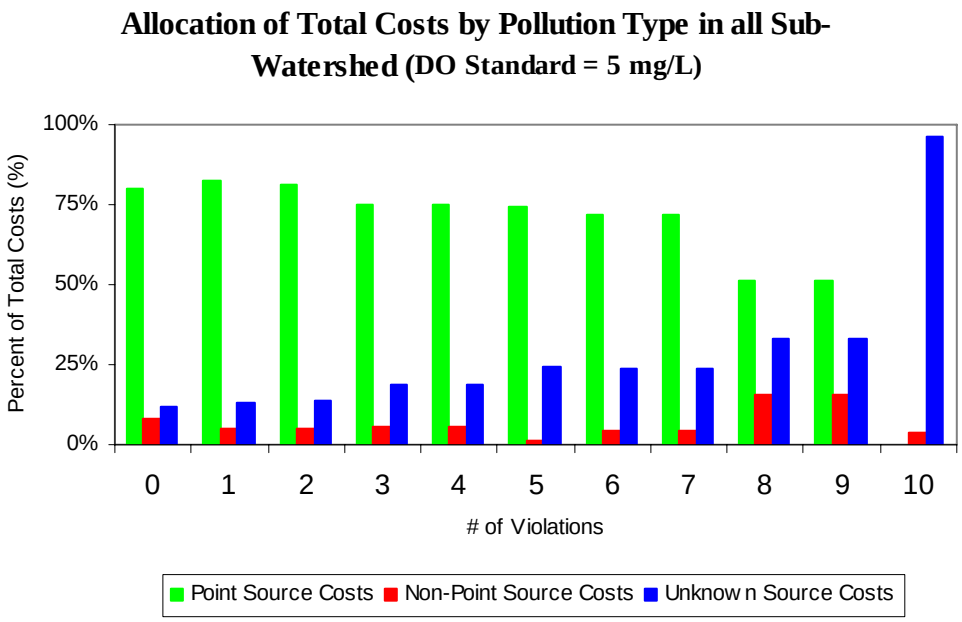


Figure 7-21. Allocation of Total Costs by Pollution Type in the Shuffled Box Complex-based Model

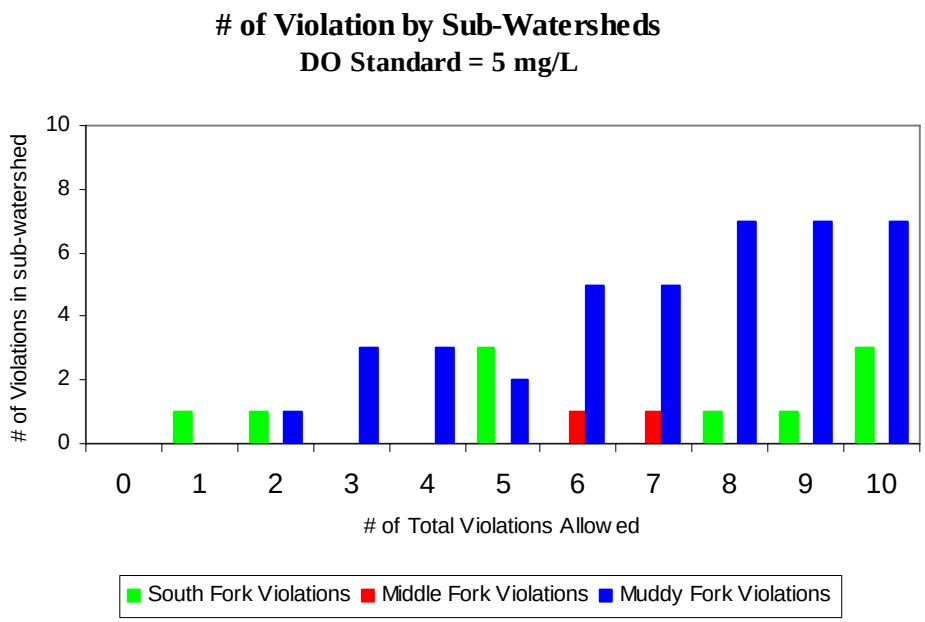


Figure 7-22. Allocation of Total Violation Days in the Shuffled Box Complex-based Model

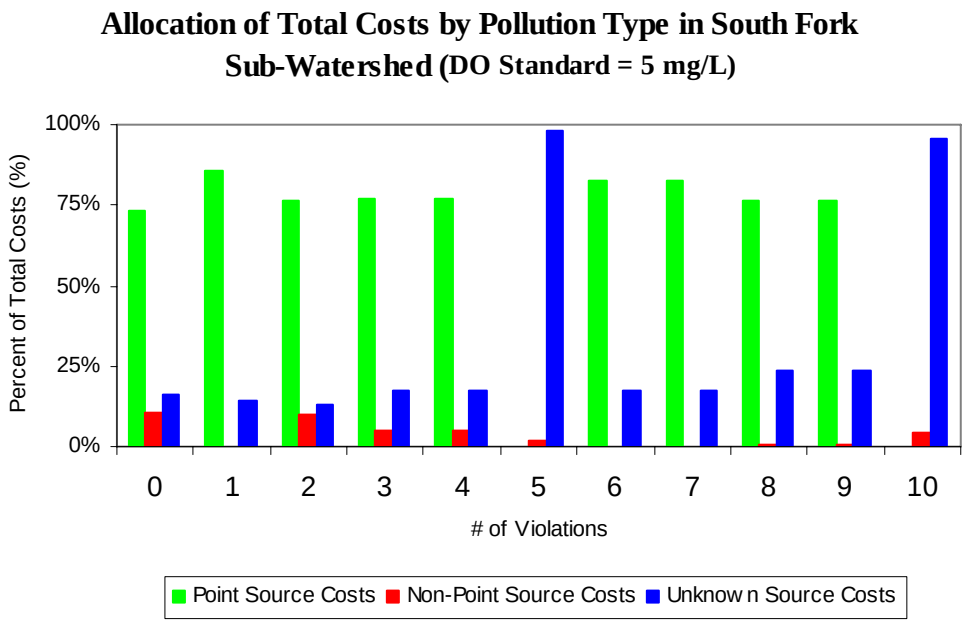


Figure 7-23. Allocation of Total Cost in South Fork by Pollution Type in the Shuffled Box Complex-based Model

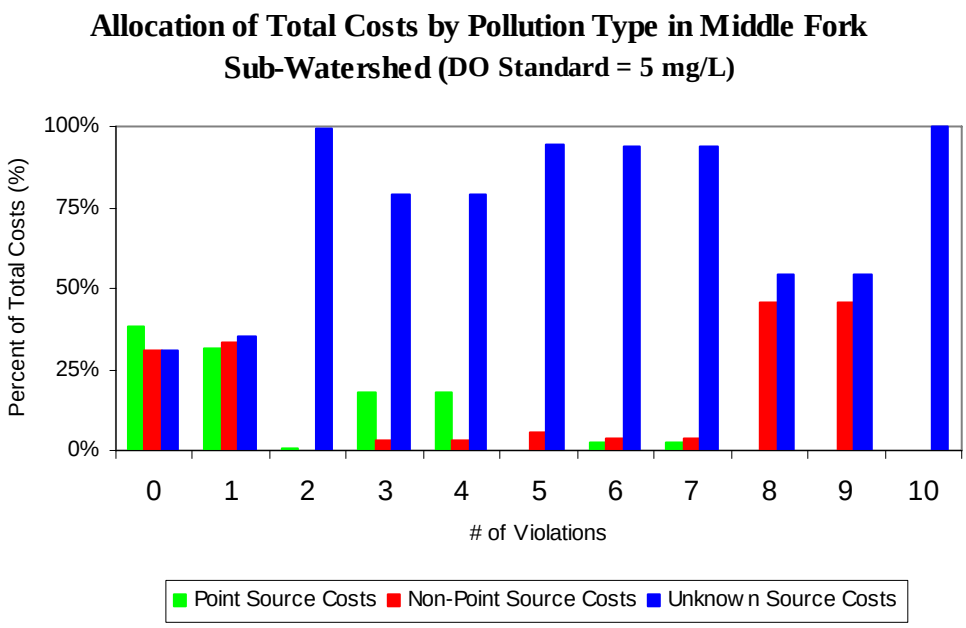


Figure 7-24. Allocation of Total Cost in Middle Fork by Pollution Type in the Shuffled Box Complex-based Model

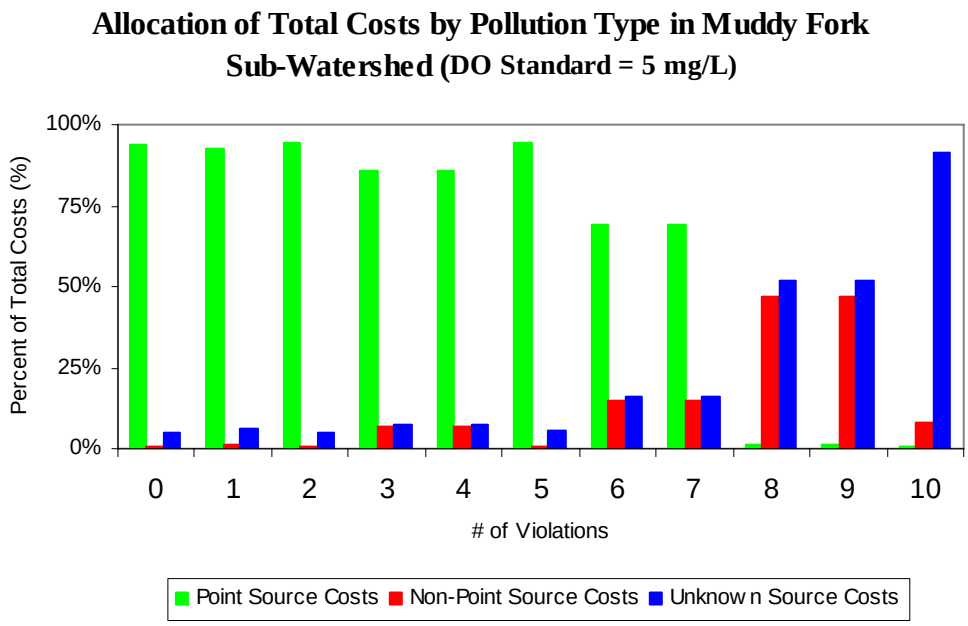


Figure 7-25. Allocation of Total Cost in Muddy Fork by Pollution Type in the Shuffled Box Complex-based Model

7.4.5.3 Discussion of Results from Water Quality-based Model

The results of the water quality-based optimal management model can be summarized as follows:

- As expected, the model is sensitive to the DO standard enforced in the simulation model. In general, as the DO standard is made more stringent (from 4 to 6 mg/L), the greater it costs to improve water quality in the sub-watersheds.
- The cost of improvements is greater in South and Muddy fork sub-watersheds for a given scenario (i.e. number of DO violations allowed and corresponding DO standard in the simulation model). This is justified by the fact that these two watersheds have proportionally more impairments than the Middle fork sub-watershed.
- Generally speaking, in the South fork sub-watersheds, the number of impairment days are driven by the point sources and leaking sewers. In the Middle fork sub-watershed, the number of impairment days are driven by non-point sources and

leaking sewers. Finally, in the Muddy fork sub-watershed, the number of impairment days is driven by a combination of all the three sources of pollution.

- The performance of the Shuffled Box Complex method is superior to GA in the optimal management model in regard to identifying least-cost solutions for a given scenario. Shuffled Box Complex method has the advantage of handling the inequality constraints explicitly in the formulation and do not require penalty functions. GAs, on the other hand, requires quite a bit of fine tuning in adjusting the parameters of the penalty functions used to handle infeasible solutions. It is possible that by further fine tuning and optimizing the penalty functions, GAs would be able to further improve in identifying the least-cost solutions.
- In terms of computational savings, the Shuffled Box Complex method in general performs better than the GA method in achieving the optimal solution in a shorter period of time. A graph of solution convergence performance (time it takes to achieve the optimal solution) for the two optimization methods is given in Figure 7-26.
- In general, the shuffling operation in the Shuffled Box Complex method helps in achieving the optimal solution quicker when compared to a model in which no shuffling is performed. When run for an extended period of time, the two models (one with the shuffling and one without the shuffling) converge to the same optimal solution. A graph of the performance of the two models for a total of 1000 generations for the water quality-based management model (DO standard of 5.0 mg/L) is given in Figure 7-27.
- The optimal management model was successful in identifying optimal management strategies that could lead to improving the DO in the streams of the Beargrass Creek watershed.

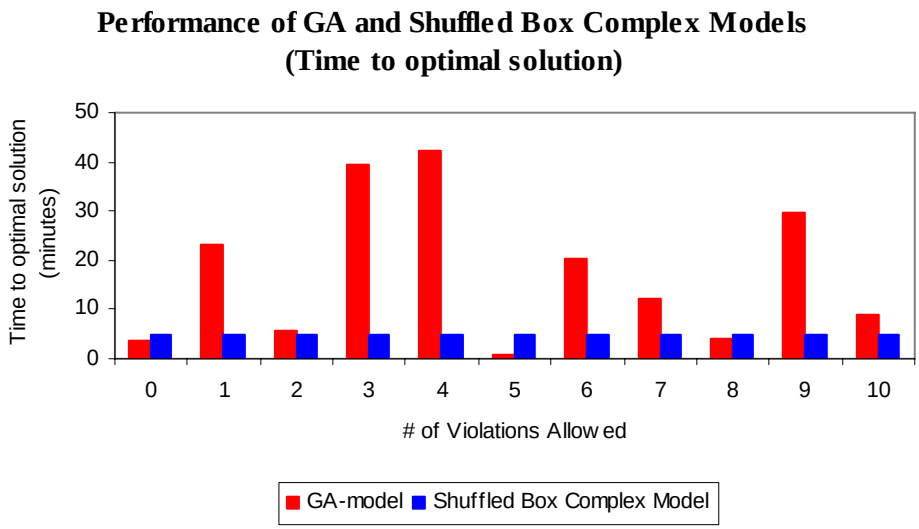


Figure 7-26. Performance of the two Optimization Methods in the Water Quality-based Management Model

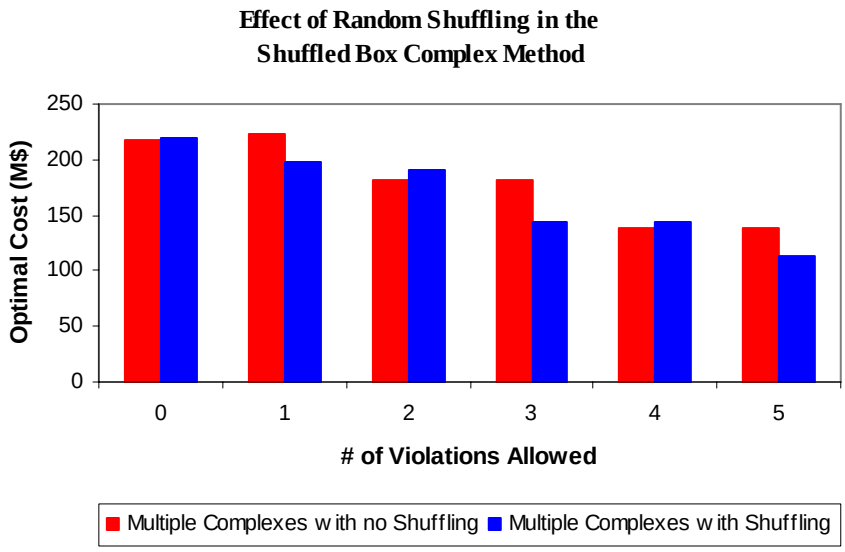


Figure 7-27. Performance of the Shuffled Box Complex Method in the Water Quality-based Management Model

7.5 Budget-based Optimal Management Model

In the budget-based formulation, the objective is to minimize the number of impairment days (i.e. DO violation days) while not exceeding a prescribed project budget. In such a formulation, the total cost of the management strategy evaluated is a constraint while the number of water quality violations constitutes the objective function. The objective function and associated constraints are given as follows in Equations 7-18 through 7-22.

7.5.1 Objective Function

The objective function for a budget-based formulation is to minimize water quality violations while satisfying the cost constraints as prescribed by a project budget. The decision variables that constitute a management strategy in the optimization framework are the same as described in the water quality-based optimal management formulation above. Mathematically, the objective function is expressed as given in Equation (7-18).

$$Minimize \quad \eta \quad = \quad \sum_{w=1}^{3}\sum_{t=1}^{267}\left[\lambda\left(X_i, Y_j\ Z_k\right)\right]_{tw} \qquad for\ all\ i, j, k \tag{7-18}$$

Where η is the number of water quality impairment days, w is the index for sub-watersheds, t is the daily time step used in the model, i is the index for point sources of pollution, j is the index for non-point sources of pollution, k is the index for other unknown or undetermined sources of pollution, $X_{i,w}$ is the decision variable for point source control in each sub-watershed, $Y_{j,w}$ is the decision variable for non-point source control in each sub-watershed, $Z_{k,w}$ is the decision variable for unknown or undetermined source control in each sub-watershed. All decision variables are defined in Figure 7-7.

7.5.2 Constraints

The objective function as described in (7-18) above is subject to three types of constraints: 1) a set of implicit system constraints, 2) a set of implicit bound constraints, and 3) a set of explicit decision variable bound constraints.

7.5.2.1 Implicit System Constraints

Similar to the water quality-based formulation described above, the inverse loading simplified deductive BOD model developed for the Beargrass Creek watershed (also described in Chapter 5) was used to represent the implicit system constraints in the budget-based optimal management model. This simple deductive model is based on the classic Streeter-Phelps (Streeter and Phelps, 1925) dissolved oxygen deficit equation. The decision variables (as given in Figure 7-7) from the optimization model ($X_{i,w}$, $Y_{j,w}$, and $Z_{k,w}$) are passed on to this simulation model which in turn calculates the effective BOD concentration (L_o) for each of the three sub-watersheds. The effective BOD concentration (L_o) calculated for each sub-watershed is then used in the forward DO model to compute a corresponding time series of DO. The mechanism of how a particular set of decision variables constituting a management strategy translates into a modified effective BOD load and subsequent DO time series is explained in detail in the water quality-based formulation in the previous section.

7.5.2.2 Implicit Bound Constraints

The implicit bound constraints include the total cost of a management strategy for the watershed under study. Since this optimal management model is budget based, an upper bound on total project budget is prescribed and the goal of the optimal management model is to select a management strategy that maximizes the water quality benefits (i.e. minimizes the number of DO impairment days) while keeping within the prescribed project budget. This may be expressed as given in Equation (7-19) as follows:

$$\sum_{w=1}^{3}\left[\left(C(X_{iw})\right) + \left(C(Y_{jw})\right) + \left(\sum_{k=1}^{n} C(Z_{kw})\right)\right] \leq \Phi \qquad (7\text{-}19)$$

Φ is the prescribed total project budget to be spent in all sub-watersheds that should not be exceeded while maximizing the water quality benefits for the watershed, w is the index number for sub-watersheds, i is the index for point sources of pollution, j is the

index for non-point sources of pollution, k is the index for other unknown or undetermined sources of pollution, n is the number of unknown or undetermined sources of pollution in each sub-watershed, $X_{i,w}$ is the decision variable for point source control in each sub-watershed, $Y_{j,w}$ is the decision variable for non-point source control in each sub-watershed, $Z_{k,w}$ is the decision variable for unknown or undetermined source control in each sub-watershed, $C(X_{i,w})$ is the cost of point source control decision variable in a sub-watershed, $C(Y_{j,w})$ is the cost of non-point source control decision variable in a sub-watershed, and $C(Z_{k,w})$ is the cost of unknown or undetermined source control decision variable in a sub-watershed.

7.5.2.3 Explicit Decision Variable Bound Constraints

The final set of bound constraints consists of explicit bounds on the decision variables in the optimization model. Mathematically, this may be expressed as given in Equations 7-20 through 7-22 as follows:

$$0 \leq X_{iw} \leq X_{\max} \qquad \forall\, i, w \qquad (7\text{-}20)$$

$$0 \leq X_{jw} \leq X_{\max} \qquad \forall\, j, w \qquad (7\text{-}21)$$

$$0 \leq X_{kw} \leq X_{\max} \qquad \forall\, k, w \qquad (7\text{-}22)$$

Where w refers to a sub-watershed and i, j, k refers to the three types of pollution sources.

7.5.3 Solution Methodology

The optimal management model is used to evaluate multiple management strategies comprising of different combinations of the 16 decision variables. The effect of these strategies is evaluated on the watershed response via the macro-level deductive dissolved oxygen (DO) simulation model. The objective of the model is to search for the optimal management strategy that minimizes the number of DO impairment days while not exceeding the specified project budget. As in the case of the water quality-based

formulation, two different optimization models are used to solve the budget-based optimal management problem. These include the GA-based optimization model and the Shuffled Box Complex-based optimization models.

7.5.4 Results of the Budget-Based Optimal Management Model

7.5.4.1 Results of the Genetic Algorithm-based Model

The objective of the budget-based optimal management model was to minimize the number of DO impairment days in the Beargrass Creek watershed while satisfying a prescribed project budget. Three different project budgets were evaluated in this management model namely $100M, $200M, and $300M. The GA-based management model was run for these project budgets to select the optimal management strategy that minimizes the number of violations. The results of the optimal management model for these three project budgets are summarized in Figure 7-28 and Table 7-16.

Table 7-16. Optimal Management Costs for Beargrass Creek Watershed (Budget-based Optimization using GA)

Project Budget (M$)	DO Impairment for 4 mg/L (# of days)	DO Impairment for 5 mg/L (# of days)	DO Impairment for 6 mg/L (# of days)
100	8	11	45
200	3	6	16
300	0	2	3

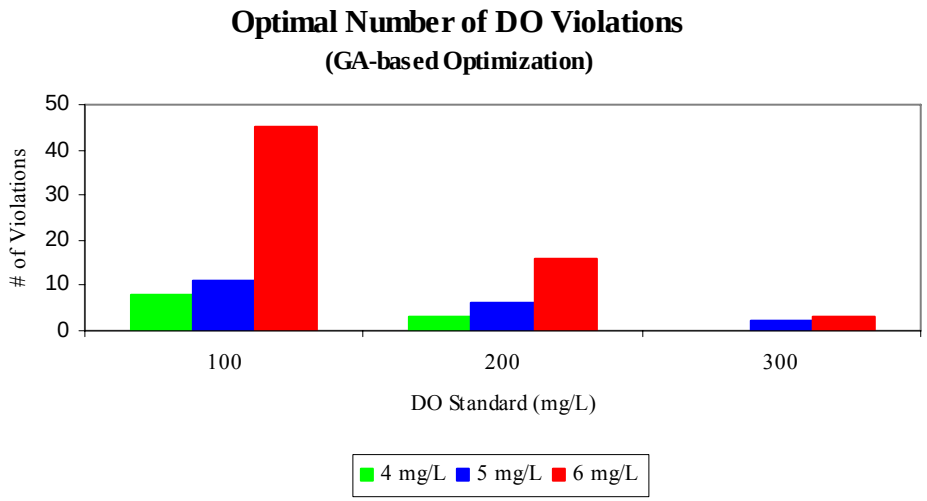


Figure 7-28. Optimal Number of Violations using GA-based Optimization

7.5.4.2 Results of the Shuffled Box Complex-based Model

The objective of the budget-based optimal management model was to minimize the number of DO impairment days in the Beargrass Creek watershed while satisfying a prescribed project budget. Three different project budgets were evaluated in this management model namely $100M, $200M, and $300M. The optimal management model for the Beargrass Creek watershed was run per the solution methodology for the Shuffled Box Complex-based optimization model. The management model utilizes the inverse-loading macro-level model for simulating the DO response in the watershed. A total of 100 feasible solutions sets are sequentially generated to form the initial complexes in the optimization model. These were partitioned into 5 different complexes, each complex consisting of 20 solution sets (vertices of the complex). The shuffling of the solution sets in each complex was performed after 100, 200, 300, and 400 generations (iterations of the model). The model was run for a total of 1000 generations (iterations). Separate models were evaluated for each of the three DO standards (4, 5, and 6 mg/L) and corresponding project budgets ($100M, $200M, $300M). The results of the Shuffled-Box Complex-based optimal management model for the Beargrass Creek watershed are summarized in Figure 7-29 and Table 7-17.

Table 7-17. Optimal Management Costs for Beargrass Creek Watershed (Budget-based Optimization using Shuffled Box Complex)

Project Budget (M$)	DO Impairment for 4 mg/L (# of days)	DO Impairment for 5 mg/L (# of days)	DO Impairment for 6 mg/L (# of days)
100	5	6	10
200	0	1	6
300	0	0	0

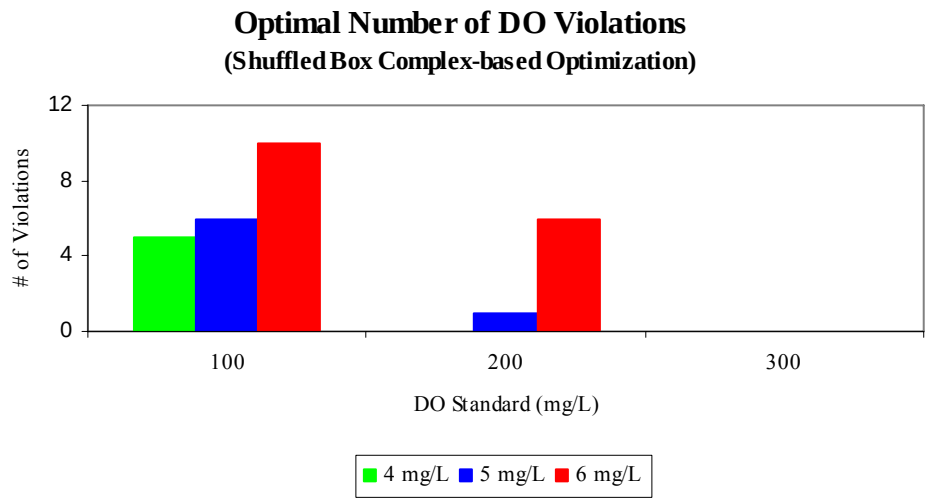


Figure 7-29. Optimal Number of Violations using Shuffled Box Complex-based Optimization

7.5.4.3 Discussion of Results from Budget-based Model

The results of the budget-based management model can be summarized as follows:

- The budget-based management model is sensitive to the DO standard enforced in the simulation model as was the case with the water quality-based management model. The number of violations increase for a prescribed budget as the DO standard is made more stringent.
- The performance of the two optimization methods differs in terms of allocating the prescribed budgets in contributing sub-watersheds for minimizing the total number of violations. In the case of Shuffled Box Complex method, the management

model is able to consume the entire budget resulting in a lower number of DO violations for the three prescribed budgets and associated DO standard. In the GA method of optimization, the management model fails to consume the entire budget resulting in a higher number of violations for the three prescribed budgets and associated DO standard.

- Overall, the results of the two budget-based optimal management models reveal that the model can be successfully applied to a watershed for allocating load reduction strategies while not exceeding a prescribed budget and minimizing the number of water quality violations. Such a model can be very beneficial for watershed managers since in most real world scenarios, it is not possible to seek a no-violation solution due to budgetary constraints and often it is required to implement capital improvement projects on priority basis as monetary funds become available. In such cases, the proposed management model can be effectively used to identify management strategies that maximize the benefits and minimize water quality violations.

CHAPTER 8
RESEARCH CONCLUSIONS AND RECOMMENDATIONS

8.1 Research Summary

This research was motivated by the challenges posed by urban watershed management due to the various sources of pollution that are responsible for impairing the water bodies. Modeling the processes occurring in such a complex watershed can also be challenging and there is a need for optimal management models for use by watershed managers to evaluate water quality management strategies leading to the selection of optimal strategies and subsequent improvement of water quality. Consequently, a comprehensive integrated watershed management methodology is developed in this research that will assist watershed managers to model and manage water quality in urban watersheds. The proposed optimal management model can be effectively used as a screening tool to evaluate least cost water quality management strategies for multiple pollution sources and sub-watersheds in an urban watershed. The computational tool is based on integration of principles from disciplines such as water quality modeling, operations research, artificial intelligence, statistics, and computer programming.

The computational methodology developed in this research consists of two major inter-connected components namely 1) a macro-level water quality simulation model, and 2) an efficient optimization model linked to the simulation model. The rationale to use macro-level simulation models in the optimal management model in this research can be justified by its benefits in a watershed management framework. Complex watersheds often require a series of deductive models to simulate the multiple processes occurring in the watershed. While such models can be expected to better reflect the true dynamics of the process or processes being modeled, such models do possess limitations. For example, such models frequently require extensive knowledge of the process being modeled, require significant efforts in calibration and verification, and can be computationally very expensive. In addition, it may be practically impossible to link such models with an optimization model in the context of a more comprehensive optimal management framework. Macro-level models on the other hand can be more manageable

computationally and depending on the type of modeling approach used may provide accuracies and precisions that approach more comprehensive deductive models. The research thus recommends that such macro-level models can be effectively incorporated into a nonlinear optimization framework for water quality management. Three different types of macro-level models were suggested for use in such a formulation and these include 1) an implicit inductive model, 2) an explicit inductive model, and 3) a simplified deductive model. Example applications were provided for two of these types: the explicit inductive and simplified deductive macro-level simulation models. The choice of a particular type depends on the particular application, available data, and the complexity of process or processes being modeled.

In the context of developing inductive models (explicit or implicit), a new mathematical technique based on genetic algorithms was developed in this research. This method is called FFSGA (Fixed Functional Set Genetic Algorithm) approach to function approximation. FFSGA can be used to develop macro-level inductive simulation models for water quality management and has the added benefit of resulting in a simple, compact, and easy to use empirical functional form for the process being modeled. FFSGA was successfully applied to a range of practical problems in water resources engineering and was found to compete favorably with other complex and nonlinear inductive modeling techniques such as genetic programming (GP) and artificial neural networks (ANNs).

Another significant component of the optimal management model developed in this research includes the optimization model. Two different optimization techniques were investigated for use in developing an optimization algorithm that is linked to the macro-level simulation model in the proposed watershed management framework. These include 1) an evolutionary method called the genetic algorithms, and 2) a modified direct search method of constrained optimization called the Shuffled Box Complex method. The use of two different classes of optimization techniques (evolutionary and direct search methods) provided a basis for testing the utility of these types of methods for use in a linked computational methodology for urban watershed management.

Lastly, the optimal management model developed in this research was tested on a real world complex urban watershed (Beargrass Creek watershed, Louisville, Kentucky) that has multiple sub-watersheds where each sub-watershed is impaired due to multiple sources of pollution. The watershed has multiple stream segments that are listed on the State's 303(d) list of impaired water bodies for pathogens and low dissolved oxygen and/or nutrient enrichment. A pathogen and dissolved oxygen (DO) TMDL (total maximum daily load) is currently under development for the watershed. The proposed optimal management model was applied to this watershed to evaluate water quality management strategies for improving the DO in the impaired streams. The optimal management model resulted in identifying the least cost management strategies to allocate water quality reductions due to point, non-point, and other unknown sources. Two different formulations of the optimal management model were applied to the Beargrass Creek watershed. These included 1) a water quality-based formulation in which the objective was to minimize costs of management strategies while satisfying prescribed water quality constraints, and 2) a budget-based formulation in which the objective was to minimize the number of water quality impairment days while not exceeding a prescribed project budget. The water quality-based management model was able to identify least cost management strategies that would need to be implemented in order to achieve all water quality goals. The budget-based approach is also beneficial since most capital improvement projects undertaken in an urban watershed rely on the capital budgets that may be available. Such a formulation would allow watershed managers strive to implement optimal management strategies while not exceeding the capital budgets available for use.

8.2 Major Conclusions of the Research

The major conclusions of this research are summarized as follows:

- A comprehensive optimal management model for integrated watershed management has the potential to assist in identifying optimal water quality management strategies for complex watersheds impaired by multiple sources of

pollution including point and non-point sources. Such a model can be constructed by linking a simulation model with an optimization model.

- A comprehensive optimal management model for integrated watershed management can be used as a practical screening tool in evaluating cost effective water quality strategies for urban watersheds.
- While deductive models may be preferred owing to their ability to better reflect the true dynamics of the process modeled, there are scenarios where this is not possible such as 1) computational expense is an issue, 2) extensive knowledge of the process being modeled is not known, 3) significant efforts are required in calibration and validation of deductive models, 4) it may not be feasible and/or practical to link such a model to an optimization model for use in an optimal management model. In such scenarios, macro-level simulation models can be effectively used in lieu of complex deductive models to represent the hydrologic and water quality processes occurring in a complex watershed and for subsequent use in the optimal management model.
- Macro-level simulation models provide an effective way to overcome some of the shortcomings of using deductive or process-based models in an optimal management model. Deductive models frequently require extensive knowledge of the process being modeled, require significant efforts in calibration and verification, and can be computationally very expensive. It may be practically not possible to link such models in a comprehensive watershed management framework. Macro-level models are relatively quick and simple and are more favorable for integration into an optimal management model.
- In theory, three different types of macro-level models can be constructed for use in the optimal management model. These include 1) an implicit inductive model, 2) an explicit inductive model, and 3) a simplified deductive model. Three different types of inductive model building techniques can be used to develop macro-level inductive simulation models. These include 1) regression, 2) artificial neural networks, and 3) genetic functions based on genetic algorithms. The flexibility and diversity of the different types of macro-level models as well as the underlying

model construction techniques makes them favorable for linkage with an optimization model in the optimal management model.

- A new genetic algorithm-based technique for function approximation called FFSGA (fixed functional set genetic algorithm) is developed in this research. FFSGA can be effectively used to develop macro-level inductive simulation models for water quality management and has the added benefit of resulting in a simple and compact empirical functional form for the process being modeled. The successful application of FFSGA to problems in water resources engineering supports that it can compete favorably with other complex and nonlinear inductive modeling techniques such as genetic programming (GP) and artificial neural networks (ANN).
- Given limited raw data, inductive models may be limited in their ability to adequately represent the cause-and-effect relationship between model inputs and outputs. For instance, the ANN-based Dissolved Oxygen (DO) model identified that such a cause-and-effect relationship between nutrients and DO could not be established. However, even in such scenarios, application of inductive models yields important information about the process or system being modeled.
- Inductive watershed models can be beneficial as they provide an insight into the effect of model inputs on model outputs and their relative sensitivity. For instance, the ANN-based DO model identified that nutrients were not the main cause of DO impairment.
- The simple deductive inverse loading model developed to simulate the dissolved oxygen (DO) and biochemical oxygen demand (BOD) dynamics in an urban watershed has the capability to model the cause and effect relationship between DO deficit and potential sources of pollution. This inverse loading model is based on the Streeter-Phelps equation (Streeter and Phelps, 1925) for modeling dissolved oxygen deficit in a water column. This novel approach is simple and the fact that it is calibrated with observed DO data makes it an effective approach. Such a model is particularly suited in scenarios where other modeling approaches fail to establish a reasonable cause-and-effect relationship between model inputs and output. An added advantage of this inverse load model is that it uses actual stream

flows and thus eliminates the use of a rainfall-runoff model. The use of rainfall-runoff models can result in a model error of 15-20%.

- A new optimization method based on modification to the Box Complex (Box, 1965) method of constrained optimization is developed called the Shuffled Box Complex method of constrained optimization. This new method introduces the concept of multiple complexes and random shuffling in the original Box Complex method and an example application to a real world complex urban watershed demonstrates that it can be successfully applied to watershed management problems with performance equal or superior to that of genetic algorithms. Like GAs, this new method is robust and diverse in its search process. The advantage of using Shuffled Box Complex over GA is that it is relatively simple and it eliminates the use of penalty functions to handle inequality constraints in the optimal management model. The use of penalty functions in using GAs for constrained optimization can be considered as a drawback as they can require extensive fine tuning and parameter estimation.
- The shuffling operation in the new Shuffled Box Complex method of optimization method generally helps in reaching the optimal solution quickly when compared to multiple complex evolutions without shuffling. When used in an optimal management model, the Shuffled Box Complex method results in significant computational savings when compared to the GA-based optimal management model due to its simple solution methodology and limited number of function calls to the simulation model.
- The proposed optimal management model provides useful insights into the dominant type of pollution sources in different sub-watersheds of a complex watershed. The management model also provide insights into pollution trade-offs between contributing watersheds and sources of pollution. The model can be effectively used to analyze the relationship between optimal cost of improvements in the watershed and the corresponding magnitude of water quality impairment in contributing watersheds. Such an analysis can be very beneficial in selecting optimal management strategies and can lead to significant cost savings.

Additionally, the proposed optimal management model provide many other added advantages and benefits for use as a management and modeling tool by watershed managers. These include the following:

- The proposed optimal management model can be effectively used to determine total maximum daily loads (TMDLs) for specified pollutants by providing for an evaluation of least-cost water quality management strategies in urban watersheds while maintaining the required water quality conditions.
- The proposed optimal management model can be used in evaluating cost effective water quality strategies for urban watersheds leading to the development of a Long Term Control Plan (LTCP) as required by EPA. Alternatively, the model can be used to support the recommendations of a LTCP.
- The proposed optimal management model can result in significant cost savings to urban communities both in watershed modeling process as well as in the identification of cost effective strategies of watershed management.

8.3 Recommendations for Future Work

With regard to the optimal management model developed in this research, the author specifically recommends the following:

- The research did not evaluate the use of implicit inductive models due to the unavailability of a calibrated deductive model for the watershed. Once such a model or suite of models are available for the Beargrass Creek watershed, it is recommended that implicit inductive models are developed based on the output of the calibrated deductive model and its utility in an optimal management framework be investigated.
- The optimal management model developed in this research provides a screening tool to evaluate management strategies for water quality management. Once a set of management strategies are selected using the model, these can be verified using a comprehensive process-based (deductive) model. It is recommended that once

the Beargrass Creek watershed water quality models are calibrated, the optimal management strategies identified in the example application should be verified using the calibrated deductive model(s).

- It is recommended that the simplified deductive dissolved oxygen model for Beargrass Creek watershed be enhanced by further refinement of the stream reaches. This can be achieved by segmenting each of the tributary stream reaches into multiple reaches for modeling the DO deficit in the watershed.
- The new Shuffled Box Complex method of constrained optimization showed great potential and promise in the example application. It is recommended that this new method be used in other applications to validate its utility as a useful tool for constrained optimization problems.
- It is recommended that the proposed Fixed Functional Set Genetic Algorithm (FFSGA) approach of function approximation be further enhanced as an inductive modeling methodology. In particular, the method should be enhanced to make it efficient for modeling functions involving a large number of inputs. The proposed method should be validated by application to problems related to hydrology and water quality management.
- Lastly, the proposed optimal management model should be applied to other complex urban watersheds for evaluating optimal water quality management strategies to validate its utility in such applications.

REFERENCES

[1]. Abadie, J. and Carpentier, J. (1969). "Generalization of the Wolfe Reduced Gradient Method to the case of Nonlinear Constraints," in Optimization, Gletcher, R. (Ed.), Academic Press, New York, 1969.

[2]. Abt, S.R. and Grigg, N.S. (1978). “An approximate method for sizing detention reservoirs.” Water Resources Bulletin, Vol. 14, No. 4, pp. 956-961.

[3]. Alvarez, L.F., Toropov, V.V., Hughes, D.C. and Ashraf, A.F. (2000). "Approximation model building using genetic programming methodology: applications". *Second ISSMO/AIAA Internet Conference on Approximations and Fast Reanalysis in Engineering Optimization.*

[4]. Anderson, J. D. (1995). Computational Fluid Dynamics: the Basics with Applications, McGraw-Hill.

[5]. Babovic, V., Keijzer, M., Aguilera, D.R., and Harrington, J. (2001). “An Evolutionary Approach to Knowledge Induction: Genetic Programming in Hydraulic Engineering”. *Proceedings of the World Water & Environmental Resources Congress*, May 21-24, 2001, Orlando, Fl. USA.

[6]. Babovic, V., (1996). *Emergence, Evolution, Intelligence: Hydroinformatics*. A.A. Balkema, Rotterdam, The Netherlands.

[7]. Babovic, V., Abbott, M. B., (1997). “The evolution of equations from hydraulic data. Part II: Applications.” *Journal of Hydraulic Research*, Vol. 35, 1997, No.3, pp.411-427

[8]. Babovic, V., Keijzer M., (2000). “Genetic programming as a model induction engine.” *Journal of Hydroinformatics*, Vol. 2, No.1, pp.35-60.

[9]. Baker, A.J. (1983). *Finite Element Computational Fluid Mechanics*. Hemisphere Publishing Corporation, New York.

[10]. Banzhaf, W., Nordin, P., Keller, R.E.., Frannkone, F.D., (1998). Genetic Programming: An Introduction: On the Automatic Evolution of Computer Programs and Its Applications, Morgan Kaufmann Publishers, Inc. and dpunkt – Verlag fur Digitale Technologie GmbH.

[11]. Bay Delta Modeling Forum (2000). *Protocols for Water and Environmental Modeling*. Bay Delta Modeling Forum (BDMF), Ad Hoc Modeling Protocols Committee, January 21, 2000.

[12]. Bay-Delta Modeling Forum (BDMF) (1997), "*Bylaws of Bay-Delta Modeling Forum*," BDMF, Richmond, CA.

[13]. Beck, M.B. (1985), *Water Quality Management: a review of the development and application of mathematical models*, Springer-Verlag, New York.

[14]. Bellman, R. (1961). *Adaptive Control Process: A Guided Tour.* Princeton University Press, Princeton, NJ.

[15]. Box, G.E.P. and Jenkins, G.M. (1976). Time Series Analysis: Forecasting and Control, 2nd ed. San Francisco: Holden Day, page 17-18.

[16]. Box, M. J. (1965). A new method for constrained optimization and a comparison with other methods. *Computer Journal,* (8), 42-52.

[17]. Brion, G.M., and Lingireddy, S. (2000) "Chapter 9 - Identification of pollution sources via neural networks." Artificial Neural Networks in Hydrology, Govindaraju, R.S., and A.Ramachandra Rao., Eds. Kluwer Academic Publishers, 179-197.

[18]. Brion, G. M., and Lingireddy, S. (1999). ‘‘A neural network approach to identify non-point sources of microbial contamination.’’ *Water Res.,* 33(14), 3099–3106.

[19]. Brion, G. M., Neelakantan, T. R., and Lingireddy, S. (2001). ‘‘Using neural networks to predict peak *Cryptosporidium* concentrations.’’ *J. Am. Water Works Assoc.,* 93(1), 99–105.

[20]. Brion, G.M., Neelakantan, T.R., and Lingireddy, S. (2002) “A Neural Network Based Classification Scheme for Sorting Sources and Ages of Fecal Contamination in Water.” *Water Research*, Vol. 36, No. 15, 3765-3774.

[21]. Brion, G., S. Lingeriddy, T.R. Neelakantan, M. Wang, R. Girones, D. Lees, A. Allard, and A. Vantarakis, (2004). Probing Norwalk-like virus presence in shellfish, using artificial neural networks. *Water Science and Technology*, Vol. 50, No. 1, pp. 125–129.

[22]. Brion, G. M., and Lingireddy, S. (2003). Artificial neural network modeling: a summary of successful applications relative to microbial water quality. *Water Science and Technology*, Vol. 47, No. 3, pp. 235–240.

[23]. Burn, D. H., and Yulianti, J. S. (2001). "Waste-load allocation using genetic algorithms." J. Water Resources Planning and Management, 127(2), 121–129.

[24]. Belegundu, A.D. and Chandrupatla, T.R. (1999). *Optimization Concepts and Applications in Engineering*. Prentice-Hall, Inc. New Jersey, USA.

[25]. Cauchy, A. (1847). “Method generale pour la resolution des systemes d’equations simultanees.” *Compt. Rend. Acad. Sci.* 25, 536-538.

[26]. Christensen, V.G., Jian, Xiaodong, and Ziegler, A.C., (2000). Regression Analysis and Real-Time Water-Quality Monitoring to Estimate Constituent Loads and

Yields in the Little Arkansas River, South-Central Kansas, 1995-99. U.S. Geological Survey Water Resources Investigations Report 00-4126, 36 p.

[27]. Christensen, V.G., Rasmussen, P.R., and Ziegler, A.C., (2002). Real-time water-quality monitoring and regression analysis to estimate constituent loads in Kansas streams [abst.], *in* Conference Program, National Environmental Monitoring Technology Conference, September 19-20, 2000, Boston, Massachusetts: Washington, D.C., U.S. Environmental Protection Agency, panel session 21.

[28]. Churchill, M.A., Elmore, H.L., and Buckingham, R.A. (1962). "Prediction of Stream Reaeration Rates." *J. San. Engr. Div. ASCE* SA4:1, Proc. Paper 3199.

[29]. Ciriani, T.A., Maione, U., and Wallis, J.R., (1977). *Mathematical Models for Surface Water Hydrology*, John Wiley & Sons, New York, NY.

[30]. Colebrook, C.F. (1939). Turbulent flow in pipes, with particular reference to the transition between the smooth and rough pipe laws. *Journal of the Institution of Civil Engineers* 11, 133-156.

[31]. Craig, E.W., Meredith, D.D., and Middletown, A.C., (1978). "Algorithm for Optimal Activated Sludge Design", ASCE Journal of the Environmental Engineering Division, December, 1978, 1101-1117.

[32]. Davidon, W.C. (1959). "Variable metric method for Minimization." AEC Res. Develop. Rep., ANL-599.

[33]. Davidson, J.W., D.A. Savic, and G.A. Walters, (1999). Method for Identification of Explicit Polynomial Formulae for the Friction in Turbulent Pipe Flow. *Journal of Hydroinformatics*, Vol. 1, No. 2, pp. 115-126.

[34]. Davis, Mike (2005). Personal communication with Project Manager of Strand Associates, Inc., Lexington, Kentucky

[35]. DeBarry, Paul A. (2004). Watersheds: Processes, Assessment, and Management. John Wiley & Sons, Inc., Hoboken, New Jersey.

[36]. DeJong, K.A. (1975). Analysis of the behavior of a class of genetic adaptive systems. Ph.D. Dissertation, University of Michigan.

[37]. Dorn, J.L. (2004). Evolutionary Algorithms to aid Watershed Management. PhD Dissertation, North Carolina State University, Raleigh, NC.

[38]. Dorn, J., Kuterdam, C., Chetan, K., Murray, T., Parandekar, A., Whangbo, A., and Ranjithan, S.R. (2001). BASINS STAR: An Evolutionary Algorithm-Based Decision Support Framework for Watershed Water Quality Management. *Proc. ASCE EWRI Conf. - Bridging the Gap: Meeting the World's Water and Environmental Resource Challenges*.

[39]. Drecourt, J.-P. (1999). Application of Neural Networks and Genetic Programming to Rainfall-Runoff Modeling. D2K Technical Report 0699-1, DHI, Copenhagen.

[40]. Drunpob, A., Chang, N.B., and Beaman, M. (2005). "Stream Flow rate Prediction using Genetic Programming Model in a Semi-Arid Coastal Watershed." *Proceedings of the 2005 World Water and Environmental Resources Congress*, Environmental and Water Resources Institute (EWRI) of the ASCE, May 15-19, 2005, Anchorage, Alaska.

[41]. Duan, Q., V. K. Gupta, and S. Sorooshian, 1993: A shuffled complex evolution approach for effective and efficient global minimization. *J. Optim. Theory Appl.,* **76,** 501–521.

[42]. Durga Rao, K. H. V., and Satish Kumar D. (2004). Spatial Decision Support System for Watershed Management. *Water Resources Management*, Vol. 18, Number 5, pp. 407 – 423.

[43]. Eberhart, R.C. and Dobbins, R.W. (1990). *Neural Network PC Tools: A Practical Guide*. Academic Press, Inc. San Diego, California.

[44]. Edwards, D. and Hamson, Mike. (1990). Guide to Mathematical Modeling. CRC Press, Boca Raton, Florida.

[45]. Environmental Protection Agency (EPA), (2005). Watershed and Water Quality Modeling Technical Support Center Website. http://www.epa.gov/athens/wwqtsc/index.html)

[46]. Environmental Protection Agency (EPA-841-R-02-001), (2002). *National Water Quality Inventory: 2000 Report*. August 2002. Office of Water (4503F), Washington DC 20460 (www.epa.gov/305b)

[47]. EPA (2002). "Costs of Urban Storm water Control." EPA-600/R-02/021, National Risk Management Research Laboratory, Office of Research and Development, U.S. Environmental Protection Agency, Cincinnati, Ohio.

[48]. Environmental Protection Agency (EPA-840-B-00-001), (2000). Liquid Assets 2000: America's Water Resources at a turning point. May 2000. Office of Water, Washington DC 20460 (www.epa.gov/water)

[49]. EPA, (1997). Compendium of Tools for Watershed Assessment and TMDL Development. EPA-841-B-97-006, U.S. Environmental Protection Agency, Office of Water, Washington, DC.

[50]. Environmental Protection Agency (EPA-832B95003), (1995). *Combined Sewer Overflows: Guidance For Nine Minimum Controls*., Washington, DC 20460. (http://www.epa.gov/npdes/pubs/owm0030.pdf)

[51]. Environmental Protection Agency (EPA). (1994). Combined Sewer Overflow Control Policy.

[52]. Esat, V., and Hall, M. (1994). "Water resources system optimization using genetic algorithms." *Hydroinformatics '94*, A. Verwey, A. Minns, V. Babovic, and C. Maksimovic, eds., Balkema, Rotterdam, The Netherlands, 225–231.

[53]. Evaldi, R.D., and Moore, B.L. (1992). Storm Water data for Jefferson County, Kentucky: U.S.Geological Survey Water Resources Investigations Report 92-638, 82 p.

[54]. Federal Register (1972-1996). "The Federal Water Pollution Control Act (Clean Water Act)." Section 33 U.S.C. §§ 1251-1387, October 18, 1972, as amended 1973-1983, 1987, 1988, 1990-1992, 1994, 1995 and 1996.

[55]. Fletcher, R. and Powell, M.J.D. (1963). "A Rapidly Convergent Descent Method for Minimization.", *Computer J*. 6, 163.

[56]. Flores, A.C., Bedient, P.B., and Mays, W.L. (1982). "Method for optimizing size and location of urban detention facilities." Proceedings of the International Symposium on Urban Hydrology, Hydraulics, and Sediment Control." University of Kentucky, Lexington, Kentucky, pp. 357-366.

[57]. Fogel, L., Owens, A., and Walsh, M. (1966). *Artificial intelligence through simulated evolution*, Wiley, New York.

[58]. Fogel, L.J. (1962), "Autonomous Automata", Industrial Research, Vol. 4, pp 14-19.

[59]. Giustolisi, O. and Savic, D.A. (2004). A Novel Genetic Programming Strategy: Evolutionary Polynomial Regression. In Liong, S-Y., K-K. Phoon and Babovic (eds.), *Proc. of the 6th International Conference on Hydroinformatics*, Vol. 1, Singapore, 21-24 June, World Scientific Pubs, New Jersey, pp 787-794.

[60]. Giustolisi, O., Savic, D.A., Doglioni, A., and Laucelli, D. (2004). Knowledge Discovery by Evolutionary Polynomial Regression, In Liong, S-Y., K-K. Phoon and Babovic (eds.), *Proc. of the 6th International Conference on Hydroinformatics*, Vol. 2, Singapore, 21-24 June, World Scientific Pubs, New Jersey, pp 1647-1654.

[61]. Goktas, R. K. and Aksoy, A. (2004). Application of Genetic Algorithms for Calibration and Verification of QUAL2E Model. *Proceedings of the 2004 World Water and Environmental Resources Congress*, ASCE, June 27-July 1, 2004, Salt Lake City, UT.

[62]. Goldberg, D. E. (1989). *Genetic Algorithms in Search, Optimization, and Machine Learning*. Addison-Wesley, Reading, Massachusetts.

[63]. Gower, A.M. (1980). Water Quality in Catchment Ecosystems. John Wiley & Sons, New York, NY.

[64]. Harrell, L.J. and Ranjithan, S.R. (1997). "Generating efficient watershed management strategies using a genetic algorithm-based method." *Proceedings of the 24th Annual Conference of the Water Resources Planning and Management Division*, ASCE, Houston, TX, April 6-9.

[65]. Haupt, R., and Haupt, S., 1998, Practical genetic algorithms: John Wiley and sons.

[66]. Hellman, A. P., and J. W. Nicklow. 2000. Optimal design of storm water inlets for highway drainage. *Proceedings of the 2000 Joint Conference on Water Resources Engineering and Water Resources Planning and Management,* ASCE. Minneapolis, MN.

[67]. Hestenes, M.R. and Stiefel, E. (1952). "Methods of Conjugate Gradients for Solving Linear Systems." *NBS Res. J.*, 49, 409-436.

[68]. Hilton, A.B. and Culver, T.B. (2000). Constraint handling for genetic algorithms in optimal remediation design. *J. Water Resources Planning and Management. ASCE* 126 **(**3) 128-137.

[69]. Holland, J. H. (1975). *Adaptation in Natural and Artificial Systems*. University of Michigan Press, Ann Arbor.

[70]. Hopfield, J.J. (1982). "Neural Networks and physical systems with emergent collective computational abilities." *Proc. Nat. Academy of Scientists*, 79:2554-2558.

[71]. Houck, Oliver A. (2002). The Clean Water Act TMDL Program: Law, Policy, and Implementation. Environmental Law Institute, Washington, D.C.

[72]. Jain, Ashu (1994). Development of a Decision Support System for Drought Characterization and Management. PhD Dissertation, Civil Engineering Department, University of Kentucky, Lexington, Kentucky.

[73]. James, W. (1890). Principles of Psychology: Briefer Course, Holt, New York.

[74]. Jarrett, L. (personal communication) (2005).

[75]. Jarrett, G. L., A. C. Downs, P. A. Grace. (1998). Continuous hydrological simulation of runoff for the Middle Fork and South Fork of the Beargrass Creek Basin in Jefferson County, Kentucky. Water-Resources Investigations Report 98-4182, 20 pp.

[76]. Jarrett, G.L. and M.J. Saffran. (1999). *Water Quality in Jefferson County: A watershed synthesis report, 1991-1998.* Prepared for the Louisville and Jefferson County Metropolitan Sewer District. 132 pp.

[77]. Jayawardena, A.W., Muttil, N., and Lee, J.H.W. (2006). "Comparative Analysis of Data-Driven and GIS-based Conceptual Rainfall-Runoff Model." *Journal of Hydrologic Engineering*, Vol. 11, No. 1, January 1, 2006.

[78]. Kentucky Division of Water (KDOW). (2004). Kentucky Administrative Regulations 401 KAR 5:031–Surface Water Standards. http://www.lrc.state.ky.us/kar/401/005/031.htm.

[79]. Kentucky Division of Water (KDOW). (2003). *2002 List of Waters for Kentucky*. Kentucky Division of Water, Frankfort, KY, 295 pp.

[80]. Koza, J. R. (1992). *Genetic Programming: On the Programming of Computers by the means of natural selection*. The MIT Press, Cambridge, Massachusetts.

[81]. Kuri-Morales, A.F. and Guti´errez-Garcia, J. (2001). P*enalty functions methods for constrained optimization with genetic algorithms: a statistical analysis*, Proc. 2nd Mexican International Conference on Artificial Intelligence, Springer-Verlag,Heidelberg,Germany,2001,pp.108–117.

[82]. Lingireddy, S., and Ormsbee, L.E., (2002) "Hydraulic Network Calibration using Genetic Optimization," *Civil and Environmental Engineering Systems,* 19(1), 13-39.

[83]. Lingireddy, S., Brion, G.M., Chandramouli, V., Neelakantan, T.R. (2003). Neural Network Modeling Software for Water and Environmental Engineering, Civil Engineering Department, University of Kentucky, Lexington, Kentucky.

[84]. Lingireddy, S. and Brion, G.M. (2004) "Chapter 1 - Artificial Neural Networks in Water Supply Engineering," *A Task Committee Report on Artificial Neural Network Applications in Water Supply Engineering*, Eds. Lingireddy and Brion, ASCE (in press).

[85]. Louisville-Jefferson County Metropolitan Sewer District (MSD) website (2005a). Available at http://www.msdlouky.org/insidemsd/wwwq/ms4/index.htm

[86]. Louisville-Jefferson County Metropolitan Sewer District (MSD) website (2005b). Available at http://www.msdlouky.org/insidemsd/wwwq/cso/index.htm

[87]. Louisville-Jefferson County Metropolitan Sewer District (MSD) website (2005c). Available at http://www.msdlouky.org/insidemsd/wwwq/sso/index.htm

[88]. Louisville-Jefferson County Metropolitan Sewer District (MSD) website (2005d). Available at http://www.msdlouky.org/insidemsd/wwwq/wma/index.htm

[89]. Lund, Jay R. and Richard N. Palmer (March 1998), "Water Resource System Modeling for Conflict Resolution," *Water Resources Update*, University Council on Water Resources, pp. 10-15.

[90]. Mays, Larry M. (1997). *Optimal Control of Hydrosystems*. Marcel Dekker, Inc. New York.

[91]. Mays, W.L. and Bedient, P.B. (1982). "Model for optimal size and location of detention." Journal of the Water Resources Planning and Management Division, ASCE, Vol. 108, No. WR3, pp. 270-285.

[92]. McCulloch, W.C. and Pitts, W. (1943). "A logical calculus of the ideas immanent in nervous activity." Bulletin of Mathematical Biophysics, Vol. 5, pp.115-133.

[93]. McKinney, D.C., Lin, M-D. (1994), "Genetic algorithm solution of ground water management models", *Water Resources Research*, Vol. 30 No.6, pp.1897-906.

[94]. Michalewicz Z. and Schoenauer M. (1996) Evolutionary Algorithms for Constrained Parameter Optimization Problems. Evolutionary Computation, 4(1):1--32.

[95]. Miettinen, K., .Makela, M.M., and Toivanen, J. (2003). *Numerical comparison of some penalty-based constraint handling techniques in genetic algorithms*, J. Global Optim. 27 (2003), no.4, 427– 446.

[96]. Minns, A.W. and Hall, M.J. (1996). "Artificial neural networks as rainfall-runoff models", *Journal of Hydrological Sciences*, **41**(3), 399-417, 1996.

[97]. Moody, L. F. (1944). Friction factors for pipe flow. Transactions of the ASME, Vol. 66.

[98]. Moyer, D.L., and K.E. Hyer. 2003. Use of the Hydrological Simulation Program - FORTRAN and bacteria source tracking for development of the fecal coliform total maximum daily load (TMDL) for Christians Creek, Augusta County, Virginia [Online]: Water Resources Investigations Report, 03-4162, USGS, Reston, VA. Available at http://www.deq.virginia.gov/tmdl/apptmdls/shenrvr/chrstnfc.pdf.

[99]. Muleta, Misgana K. (2003). A decision support system for the management of non-point source pollution from watersheds. PhD Dissertation, Southern Illinois University, Carbondale, Illinois.

[100]. Mujumdar, P. P., and V. V. R. Subba Rao, (2004) "Fuzzy Waste Load Allocation Model: A Simulation-Optimization Approach", Journal of Computing in Civil Engineering. Vol. 18, No. 2, pp. 120-131.

[101]. National Research Council (NRC). 2001. *Assessing the TMDL approach to Water Quality Management*. Report to the Committee to Assess the Scientific Basis of the Total Maximum Daily Load Approach to Water Pollution Reduction. National Academy of Sciences, Washington, D.C. September 2001.

[102]. Neelakantan, T.R., Lingireddy, S., and Brion, G.M., (2002). Relative performance of different ANN training algorithms in predicting protozoa concentration in surface waters, *ASCE Journal of Environmental Engineering*, 128(6), 533-542.

[103]. Neelakantan, T.R, Brion, G.M., and Lingireddy, S. (2001) "Neural network modeling of *Cryptosporidium* and *Giardia* concentrations in the Delaware River, USA", *Water Science and Technology*, Vol. 43, No. 12, pp 125-132.

[104]. Nelder, J. A. and Mead, R. (1965) A simplex algorithm for function minimization. *Computer Journal* **7**, 308–313.

[105]. Nestorov, Ivan S., Hadjitodorov, S.T., Petrov, I., and Rowland, Malcolm (1999). "Empirical Versus Mechanistic Modeling: Comparison of an Artificial Neural Network to a Mechanistically Based Model for Quantitative Structure Pharmacokinetic Relationships of a Homologous Series of Barbiturates." *AAPS Pharmsci* 1999; 1 (4) article 17 (http://www.pharmsci.org)

[106]. Nicklow, J.W. (2000). Discrete-time optimal control for water resources engineering and management. Water International, International Water Resources Assoc. 25(1): 89-95.

[107]. Nicklow, J.W. and Mays L.W. (2000). "Optimal control of reservoir release to minimize sedimentation in rivers and reservoirs." *J. of the American Water Resources Association*, 37(1): 197-211.

[108]. Nishikava, T. (1998). “Water Resources optimization model for Santa Barbara, California.” *J. Water Resources Planning and Management. ASCE* 124 **(**5) 252-263.

[109]. O’Connor, D.J. and Dobbins. (1958). “Mechanism of Reaeration in Natural Stream.” *Trans. Am. Soc. Civil Engin*. 123:641-666.

[110]. Oliveira, R. and D.P. Loucks. 1997. .Operating Rules for Multireservoir Systems. Water Resources Research 33, No.4: 839.852.

[111]. Ormsbee, L. E., and Reddy, S. L. (1995). "Nonlinear heuristic for pump operations." Journal of Water Resources Planning and Management, 121(4), 302-309.

[112]. Ormsbee, L. E. (1986). "A Nonlinear Heuristic for Applied Problems in Water Resources." *Proceedings of Seventeenth Annual Modeling and Simulation Conference*, University of Pittsburgh, Pittsburgh, Pennsylvania.

[113]. Ormsbee, L.E., Delleur, J.W., and Houck, M.H. (1984). “Development of a general planning methodology for storm water management in urban watersheds”, TR-163, Purdue University Water Resources Research Center, West Lafayette, Indiana, March 1984.

[114]. Ormsbee, L.E. (1985). “OPNET: A nonlinear algorithm for Hydraulic Networks”, Computer Applications in Water Resources, American Society of Civil Engineers, New York, New York, June 1985, 739-748.

[115]. Ormsbee, L.E. (1983). Systematic Planning of Dual Purpose Detention Basins in Urban Watersheds. PhD Dissertation, Purdue University, West Lafayette, Indiana, USA.

[116]. Owens, M., Edwards, R., and Gibbs, J. (1964). Some Reaeration Studies in Streams. *Int. J. Air Water Poll*. 8:469-486.

[117]. Pinder, G.F. and Wiggert, D.C. (1991). Mechanics of Fluids. Prentice Hall, New Jersey, p.154-155.

[118]. Powell, M. J. D. (1964): An efficient method for finding the minimum of a function of several variables without calculating derivates. Computer Journal 7: 155-162.

[119]. Radwan, M., Willems, P., El-Sadek, A., and Berlamont, J. (2003) "Modeling of dissolved oxygen and biochemical oxygen demand in river water using a detailed and a simplified model." *Intl. J. River Basin Management* Vol. 1, No. 2 (2003), pp. 97–103.

[120]. Rogers, D. and Hopfinger, A.J. (1994). Application of genetic function approximation to quantitative structure-activity relationships and quantitative structure-property relationships. *J. Chem. Inf. Comput. Sci., 34*, 854-866.

[121]. Reddy, J.N. (1993). *An Introduction to the Finite Element Method*, 2nd Edition, McGraw Hill Inc. New York.

[122]. Reid, J. (1971). "On the Method of Conjugate Gradients for the Solution of Large Sparse Systems of Linear Equations." Proceedings of the Oxford Conference of the Institute of Mathematics and its Applications, April, 1970, Academic Press, London, pp. 231-254.

[123]. Reis, L.F.R., Porto, R.M. and Chaudhry, F.H. "Optimal Location of Control Valves in Pipe Networks by Genetic Algorithm." *J. Water Resources Planning and Management*, ASCE, 123(6), 317-320, 1997.

[124]. Reklaitis, G. V., A. Ravindran and K. M. Ragsdell, *Engineering Optimization: Methods and Applications*, John Wiley and Sons, Inc., New York (1983).

[125]. Ritzel, B.J., J.W. Eheart, and S. Ranjithan, Using genetic algorithms to solve a multiple objective groundwater pollution containment problem, *Water Resources Research*, 30(5), 1589-1603, 1994.

[126]. Rosenbrock, H. H. (1960). An automatic method for finding the greatest or least value of a function. *Computer. Journal,* (3), 175–184.

[127]. Rosenblatt, F. (1958). "The Perceptron: A Probabilistic Model for Information Storage and Organization in the Brain." Psychological Review, Vol. 65, pp.386-408.

[128]. Ruhl, K. and Jarrett, G. L. (1999). Processes affecting dissolved-oxygen concentrations in the lower reaches of Middle Fork and South Fork Beargrass Creek, Jefferson County, Kentucky. U.S. Geological Survey Water Resources Investigations Report 98-4218, 53p.

[129]. Rumelhart, D.E., McClelland, J.L., and the PDP Research Group (1986). *Parallel Distributed Processing – Volume1: Foundations*, the MIT Press, Cambridge, MA.

[130]. Sarker, R., Mohammadian, M., and Yao, X., editors (2002). *Evolutionary Optimization*. Kluwer Academic Publishers.

[131]. Savic, D.A., G.A. Walters and Davidson, J.W. (1999). "A Genetic Programming Approach to Rainfall-Runoff Modeling." *Water Resources Management*, Vol. 13, No. 3, pp. 219-231.

[132]. Savic DA, Walters GA (1997) Genetic algorithms for least-cost design of water distribution networks. *Journal of Water Resources Planning and Management*, ASCE 123(2):67–77.

[133]. Schwefel, H.P. (1981). *Numerical optimization of computer models*. John Wiley & Sons, New York, NY.

[134]. Schwefel, H.P. (1995). *Evolution and optimum seeking.* Wiley, New York, NY.

[135]. Schoenbaum, Thomas J., Rosenberg, Ronald H., and Doremus, Holly D. (2002). Environmental Policy Law: Problems, Cases, and Readings. 4th Edition. Foundation Press, New York.

[136]. Sengupta, R., Bennett, D.A., Beaulieu, J., and Kraft, S.E. (2000). "Evaluating the impact of policy-induced land use management practices on non-point source pollution using a spatial decision support system." *Water International*, 25(3): 437-445.

[137]. Shi, L.M., Fan, Y., Myers, T.G., O'Connor, P.M., Paull, K.D., Friend, S.H., and Weinstein, J.N. (1998). Mining the NCI Anticancer Drug Discovery Database: Genetic Function Approximation for the QSAR Study of Anticancer Ellipticine Analogues, *J. Chem. Inf. Comput. Sci., 38*, 189-199.

[138]. Sinha, N.K. (1991). *Linear Systems*. John Wiley & Sons, New York.

[139]. Spendley, W., Hext, G. R., Himsworth, F. R. Sequential application of simplex designs in optimization and evolutionary operation. Technometrics 4(1962):4 441-461.

[140]. Srivastava, P., Hamlet, J.M., Robillard, P.D., and Day, R.L. (2002). "Watershed optimization of best management practices using ANNAGNPS and a genetic algorithm." *Water Resources Res*., 38(3): 1-14.

[141]. Stasa, F.L., (1985). *Applied Finite Element Analysis for Engineers*. Holt, Rinehart and Winston, New York.

[142]. Streeter, H.W. and Phelps, E.B. (1925). "A Study of the Pollution and Natural Purification of the Ohio River III. Factors concerning the Phenomena of Oxidation and Reaeration." U.S. Public Health Service, Pub. Health Bulletin No. 146, February 1925. Reprinted by U.S., DHEW, PHA, 1958.

[143]. Suen, Jian-Ping, and Eheart, J.W. (2003). Evaluation of Neural Networks for Modeling Nitrate Concentrations in Rivers. J. Water Resources Planning and Management, Volume 129, Issue 6, pp. 505-510.

[144]. Swamee, P. K., and Jain, A. K. (1976). "Explicit equations for pipe-flow problems". J. Hydraul. Div., Am. Soc. Civil. Eng., 102(5), 657–664.

[145]. Tetra Tech Inc. (2005). Quality Assurance Project Plan (QAPP) for Beargrass Creek Water Quality Tool and TMDLs Development. Prepared for Louisville and Jefferson County Metropolitan Sewer District (MSD). Tetra Tech Inc. Fairfax, Virginia.

[146]. Thomann, R. V., and J. A. Mueller. 1987. Principles of surface water quality modeling and control. Harper & Row, New York, New York.

[147]. Tufail, M. and Ormsbee, L.E. (2006). "*A Fixed Functional Set Genetic Algorithm (FFSGA) Approach for Function Approximation*." Accepted for publication in the IWA Journal of Hydroinformatics (in press).

[148]. Tufail, M. and Ormsbee, L.E. (2005c). "The utility of Inductive models using Artificial Intelligence (AI) Techniques for Water Quality Management in a TMDL Framework." *Proceedings of the* W*ater Environment Federation (WEF) TMDL 2005 Specialty Conference,* Philadelphia, Pennsylvania, June 26-29, 2005.

[149]. Tufail, M. and Ormsbee, L.E. (2005a). Optimal Load Allocations by Linkage of Evolutionary Optimization Algorithms with Inductive Models of Watershed Response. *Proceedings of* the *ASCE World Water and Environmental Resources Congress Annual Conference,* Anchorage, Alaska, May 15-19, 2005.

[150]. Tufail, M. and Ormsbee, L.E. (2005b). Development of Inductive Receiving Water Model for Application in TMDLs. *Proceedings of* the *ASCE World Water and*

Environmental Resources Congress Annual Conference, Anchorage, Alaska, May 15-19, 2005

[151]. Tufail, M., Ormsbee, L.E. and Teeagavarapu, R. (2004). A Comparison of two Artificial Intelligence (AI) Techniques to develop Functional Relationships for Water Quality Loadings. *Proceedings of the ASCE World Water and Environmental Resources Congress Annual Conference,* Salt Lake City, Utah, June 28-July 1, 2004

[152]. Tufail, Mohammad (1995). CE 790 Special Research Problems in Civil Engineering, *Galerkin-Least Squares Finite Element Method One Dimensional Unsteady Open Channel Flow Model*, Master's Research Report, Department of Civil Engineering, University of Kentucky, Lexington, KY, May 1995.

[153]. U.S. Department of Justice (2005). Press Release on April 25, 2005 (http://www.usdoj.gov/opa/pr/2005/April/05_enrd_213.htm)

[154]. U.S. House of Representatives, the Subcommittee on Water Resources and Environment Hearing on the Future of the TMDL Program: How to Make TMDLs Effective Tools for Improving Water. (http://www.house.gov/transportation/water/11-15-01/11-15-01memo.html)

[155]. Vrugt JA, Gupta HV, Bouten W, Sorooshian S. (2003). A shuffled complex evolution Metropolis algorithm for optimization and uncertainty assessment of hydrologic model parameters. *Water Resources Research* 39(8): 1201.

[156]. Vrugt, J.A., Gupta, H.V., Bastidas, L.A., Bouten, W., Sorooshian, S. (2003). Effective and efficient algorithm for multi-objective optimization of hydrologic models. Water Resources Research. 39 (8), 5.1–5.19.

[157]. Wang, Q.J. 1991. "The genetic algorithm and its application to calibrating conceptual rainfall-runoff models." Water Resources Research, 27:2467–2471.

[158]. Wardlaw R, Sharif M (1999) Evaluation of genetic algorithms for optimal reservoir system operation. J Water Resources Planning and Management ASCE 125(1):25–33.

[159]. Wu, J.S., Han, J., Annambhotla, S., and Bryant, S. (2005). "Artificial Neural Networks for Forecasting Watershed Runoff and Stream Flows." Journal of Hydrologic Engineering, ASCE, Vol. 10, No. 3, pp. 216-222.

[160]. Yeniay, O. (2005). Penalty Function Methods for Constrained Optimization with Genetic Algorithms, *Mathematical and Computational Applications*, Vol. 10, No. 1, pp. 45-56, 2005.

[161]. Yeniay, O. (2005). A Comparative Study on Optimization methods for the constrained nonlinear programming problems. Mathematical Problems in Engineering 2005:2(2005)165–173.

[162]. Zealand, C. M., Burn, D. H., and Simonovic, S. P. (1999). "Short-term stream flow forecasting using artificial neural networks." *Journal of Hydrology*, 214, 32–48.

[163]. Zechman, E.M. (2005). Improving Predictability of Simulation Models using Evolutionary Computation-Based Methods for Model Error Correction. PhD Dissertation, North Carolina State University, Raleigh, NC.

[164]. Zhen, X.J. and Yu, S.L. (2002). "Optimization of best management practices (BMPs) placement at the watershed scale." *Proceedings of the 2002 Conference of the Environmental and Water Resources Institute*, ASCE, Roanoke, VA, May 19-22.

[165]. Zurada, J.M. (1992), Introduction to Artificial Neural Systems. Boston, MA.

VITA

Mohammad Tufail was born in Swabi in the North West Frontier Province of Pakistan on March 15, 1971. After completing High School in 1988 from Cadet College Kohat (Pakistan), he joined the NWFP University of Engineering and Technology in Peshawar, Pakistan to pursue a BS degree in Civil Engineering. After completing two years of education at the University, he moved to the University of Kentucky in Lexington, Kentucky (USA) as a transfer student pursuing a Bachelor's degree in Civil Engineering in May 1991. He was awarded a BS in Civil Engineering degree in May 1993 and MS in Civil Engineering degree in August 1995 at the University of Kentucky. After completing his Master's degree at the University of Kentucky, he was employed by Strand Associates Inc. (Top 200 Environmental Engineering Design Firm)) in August 1995 as a water resources and environmental engineer in their Lexington office. In March 2000, he moved to Charlotte, North Carolina and worked as a water resources engineer for Camp Dresser and McKee (CDM) Inc. (a global environmental engineering consulting firm) till March 2001. In March 2001, he moved back to Lexington, Kentucky, and joined Strand Associates Inc. as a Project Manager working on projects in the area of water resources and environmental engineering.

In January 2003, he joined the University of Kentucky to pursue a PhD in Civil Engineering. He is a candidate for PhD in Civil Engineering specializing in the modeling and management of water resources and environmental systems.

Mr. Tufail is a registered professional engineer in the State of Kentucky since 1999 and has worked on several key infrastructure projects related to planning and design of water resources, and environmental systems during his practice as a professional engineer. Mr. Tufail has authored numerous publications including conference proceedings, journal papers, and technical reports.

Mohammad Tufail

May 4, 2006