Effective Modeling of Nutrient Losses and Nutrient Management Practices in an Agricultural and Urbanizing Watershed

Yingmei Liu

Dissertation submitted to the faculty of the
Virginia Polytechnic Institute and State University
in partial fulfillment of the requirements for the degree of

Doctor of Philosophy
in
Civil Engineering

Adil N. Godrej, Chair
Thomas J. Grizzard
John C. Little
Theo Dillaha

December 5, 2011
Manassas, Virginia

Keywords: Watershed model, HSPF, PQUAL, AGCHEM, sensitivity analysis, water quality model, CE-QUAL-W2

Effective Modeling of Nutrient Losses and Nutrient Management Practices in an Agricultural and Urbanizing Watershed

Yingmei Liu

(ABSTRACT)

The Lake Manassas Watershed is a 189 km^2 basin located in the Northern Virginia suburbs of Washington, DC. Lake Manassas is a major waterbody in the watershed and serves as a drinking water source for the City of Manassas. Lake Manassas is experiencing eutrophication due to nutrient loads associated with agricultural activities and urban development in its drainage areas. Two watershed model applications using HSPF, and one receiving water quality model application using CE-QUAL-W2, were linked to simulate Lake Manassas as well as its drainage areas: the Upper Broad Run (126.21 km^2) and Middle Broad Run (62.79 km^2) subbasins. The calibration of the linked model was for the years 2002-05, with a validation period of 2006-07.

The aspects of effective modeling of nutrient losses and nutrient management practices in the Lake Manassas watershed were investigated. The study was mainly conducted in the Upper Broad Run subbasin, which was simulated with an HSPF model. For nutrient simulation, HSPF provides two algorithms: PQUAL (simple, empirically based) and AGCHEM (detailed, process-based). This study evaluated and compared the modeling capabilities and performance of PQUAL and AGCHEM, and investigated significant inputs and parameters for their application. Integral to the study was to develop, calibrate and validate HSPF/PQUAL and HSPF/AGCHEM models in the Upper Broad Run subbasin.

“One-variable-at-a-time” sensitivity analysis was conducted on the calibrated Upper Broad Run HSPF/PQUAL and HSPF/AGCHEM models to identify significant inputs and parameters for nutrient load generation. The sensitivity analysis results confirmed the importance of accurate meteorological inputs and flow simulation for effective nutrient modeling. OP (orthophosphate phosphorus) and NH_4-N (ammonium nitrogen) loads were sensitive to PQUAL parameters describing pollutant buildup and washoff at land surface. The significant PQUAL parameter for

Ox-N (oxidized nitrogen) load was groundwater nitrate concentration. For the HSPF/AGCHEM model, fertilizer application rate and time were very important for nutrient load generation. NH_4-N and OP loads were sensitive to the AGCHEM parameters describing pollutant adsorption and desorption in the soil. On the other hand, plant uptake of nitrogen played an important role for Ox-N load generation.

A side by side comparison was conducted on the Upper Broad Run HSPF/PQUAL and HSPF/AGCHEM models. Both PQUAL and AGCHEM provided good-to-reasonable nutrient simulation. The comparison results showed that AGCHEM performed better than PQUAL for OP simulation, but PQUAL captured temporal variations in the NH_4-N and Ox-N loads better than AGCHEM. Compared to PQUAL, AGCHEM is less user-friendly, requires a lot more model input parameters and takes much more time in model development and calibration. On the other hand, use of AGCHEM affords more model capabilities, such as tracking nutrient balances and evaluating alternative nutrient management practices.

This study also demonstrated the application of HSPF/AGCHEM within a linked watershed-reservoir model system in the Lake Manassas watershed. By using the outputs generated by the HSPF/AGCHEM models in the Upper Broad Run and Middle Broad Run subbasins, the Lake Manassas CE-QUAL-W2 model adequately captured water budget, temporal and spatial distribution of water quality constituents associated with summer stratification in the lake. The linked model was used to evaluate water quality benefits of implementing nutrient management plan in the watershed. The results confirmed that without the nutrient management plan OP loads would be much higher, which would lead to OP enrichment and enhanced algae growth in Lake Manassas.

Acknowledgements

I am extremely grateful to my advisor Adil N. Godrej for his constant inspiration, support and help. I would also like to thank my committee members, Thomas J. Grizzard, John C. Little, and Theo Dillaha, for their valuable advice and encouragement.

I have a wonderful time and enjoy working with all the people at the Occoquan Watershed Monitoring Laboratory. Special thanks to Barb Angelotti and Alicia Tingen for always being encouraging and supportive. And, I want to thank Harry Post, Dongmei Wang and all other field and laboratory staff for collecting and analyzing water quality samples, which provided a solid data support for the research.

I would like to express sincere appreciation to Mr. Normand Goulet, Ms. Evelyn Mahieu, Ms. Traci Kammer Goldberg, Mr. Greg Prelewicz, my good friend Niffy Saji and other people who oversaw the Occoquan Model project, which provided continuous funding to make my Ph.D studies possible. In addition, I want to thank two nutrient management specialists from Fauquier County, Jay Marshall and Tim Ohlwiler, for their recommendations and helps in developing manure and fertilizer related inputs.

Above all, I want to thank my family for their unconditional love and support throughout my life, especially my parents, Zhaoli Liu and Xueqiu Sun. Thanks so much to my husband Yu Qiao and my daughter Amy Qiao, for always being there for me. I could not have made it without all of you in my life.

Table of Contents

Chapter 1. Introduction..1
1.1 Background and Motivation 1
1.2 Research Goal and Objectives 2
1.3 Dissertation Outline 3

Chapter 2. Literature Review 6
2.1 Watershed Models 6
2.2 Receiving Water Quality Models 13
2.3 Linked Watershed and Receiving Water Quality Model Applications 15
2.4 Sensitivity Analysis Methods 17
2.5 References.. 20

Chapter 3. Sensitivity Analysis, Calibration and Validation of a Watershed Model Application using HSPF with the Nutrient Algorithm PQUAL in Upper Broad Run Watershed, Virginia...26
3.1 Abstract.. 26
3.2 Introduction.. 27
3.3 Materials and Methods.. 30
3.3.1 Study Area 30
3.3.2 Model Development..32
3.3.3 Model Calibration and Validation..35
3.3.4 Sensitivity Analysis..36
3.4 Results and Discussion 36
3.4.1 Model Calibration and Validation Results..37
3.4.2 Sensitivity Analysis Results..42
3.5 Conclusions.. 51
3.6 References.. 53

Chapter 4. Application and Sensitivity Analysis of a Watershed Model Application using HSPF with the Nutrient Algorithm AGCHEM in Upper Broad Run Watershed, Virginia...56
4.1 Abstract.. 56
4.2 Introduction.. 57
4.3 Materials and Methods.. 60
4.3.1 Study Area 60
4.3.2 Model Development..61
4.3.3 Model Calibration and Validation..74
4.3.4 Sensitivity Analysis..74
4.4 Results and Discussion 76
4.4.1 Model Calibration and Validation Results..76
4.4.2 Sensitivity Analysis Results..80
4.5 Conclusions.. 89

4.6 References 91

Chapter 5. Comparison of two Nutrient Simulation Algorithms of HSPF in Upper Broad Run Watershed, Virginia 93
- 5.1 Abstract 93
- 5.2 Introduction 94
- 5.3 Materials and Methods 96
  - 5.3.1 Study Area 96
  - 5.3.2 Model Description 98
  - 5.3.3 Model Performance Evaluation 107
- 5.4 Results and Discussion 107
  - 5.4.1 Nutrient Load Comparison Results 107
  - 5.4.2 Nutrient Concentration Comparison Results 115
- 5.5 Summary and Conclusions 123
- 5.6 References 125

Chapter 6. Evaluation of Nutrient Management Plans Using a Linked Watershed-Reservoir Model 128
- 6.1 Abstract 128
- 6.2 Introduction 129
- 6.3 Materials and Methods 131
  - 6.3.1 Study Area 131
  - 6.3.2 Approach Used to Link the Watershed-Reservoir Model 134
  - 6.3.3 Development of Pre-BMP scenario 143
- 6.4 Results and Discussion 144
  - 6.4.1 Lake Manassas CE-QUAL-W2 Model Calibration and Validation Results 145
  - 6.4.2 Pre-BMP Scenario Analysis Results 154
- 6.5 Conclusions 158
- 6.6 References 160

Chapter 7. Evaluating HSPF Performance of Flow and Sediment Prediction at Multiple Watershed Segmentations in Upper Broad Run Watershed, Virginia 163
- 7.1 Abstract 163
- 7.2 Introduction 164
- 7.3 Study Site 167
- 7.4 Model Description and Methods 168
  - 7.4.1 Brief Description of HSPF 168
  - 7.4.2 HSPF Applications in the Upper Broad Run Watershed 169
  - 7.4.3 Model Performance Evaluation of Flow and Sediment Simulation 175
- 7.5 Results and Discussion 176
  - 7.5.1 Flow Calibration and Prediction at Stream Station ST70 177
  - 7.5.2 Sediment Calibration and Prediction at Stream Station ST70 182
- 7.6 Conclusions 186
- 7.7 References 187

Chapter 8. Conclusions and Recommendations 191
8.1 Summary.. 191
8.1.1 First Objective..194
8.1.2 Second Objective 195
8.1.3 Third Objective 197
8.2 Recommendations... 199

References Cited..201

Appendix. Nutrient Inputs for HSPF/AGCHEM Applications in Lake Manassas Watershed, Virginia 210

List of Figures

Figure 3-1: Location of Upper Broad Run Watershed, Showing Major Streams, Stream Stations and Rain Gauges in the Occoquan Watershed 31

Figure 3-2: Nutrient Simulation by PQUAL 34

Figure 3-3: Segmentation of the Upper Broad Run Watershed 34

Figure 3-4: Sensitivity Index (*S*) of Average Seasonal Flow to HSPF/PQUAL Inputs and Parameters 46

Figure 3-5: Sensitivity Index (*S*) of Average Seasonal TSS Loading to HSPF/PQUAL Inputs and Parameters 48

Figure 3-6: Sensitivity Index (*S*) of Average Seasonal OP Loading to HSPF/PQUAL Inputs and Parameters 49

Figure 3-7: Sensitivity Index (*S*) of Average Seasonal NH_4-N Loading to HSPF/PQUAL Inputs and Parameters 50

Figure 3-8: Sensitivity Index (*S*) of Average Seasonal Ox-N Loading to HSPF/PQUAL Inputs and Parameters 51

Figure 4-1: Location of Upper Broad Run Watershed, Showing Major Streams, Stream Stations and Rain Gauges in the Occoquan Watershed 61

Figure 4-2: Segmentation of the Upper Broad Run Watershed 62

Figure 4-3: Flow Diagram for Nitrogen Reactions by NITR 64

Figure 4-4: Flow Diagram for Phosphorus Reactions by PHOS 64

Figure 4-5: High and Low Tillage Cropland Distributions in Fauquier County 65

Figure 4-6: Sensitivity Index (*S*) of Average Seasonal OP Loading to HSPF/AGCHEM Inputs and Parameters 85

Figure 4-7: Sensitivity Index (*S*) of Average Seasonal NH_4-N Loading to HSPF/AGCHEM Inputs and Parameters 87

Figure 4-8: Sensitivity Index (*S*) of Average Seasonal Ox-N Loading to HSPF/AGCHEM Inputs and Parameters 88

Figure 5-1: Location of Upper Broad Run Watershed, Showing Major Streams, Stream Stations and Rain Gauges in the Occoquan Watershed................................97

Figure 5-2: Segmentation of the Upper Broad Run Watershed..99

Figure 5-3: Flow Diagram for Nitrogen Reactions by NITR 101

Figure 5-4: Flow Diagram for Phosphorus Reactions by PHOS 101

Figure 5-5: Nitrogen Inputs from Fertilizer and Manure..105

Figure 5-6: Phosphorus Inputs from Fertilizer and Manure 106

Figure 5-7: Comparison of Annual and Seasonal NH_4-N Loads, 2002-2007.................109

Figure 5-8: Comparison of Annual and Seasonal Ox-N Loads, 2002-2007....................110

Figure 5-9: Comparison of Monthly NH_4-N Loads, 2002-2007.....................................112

Figure 5-10: Comparison of Monthly Ox-N Loads, 2002-2007.....................................112

Figure 5-11: Comparison of Annual and Seasonal OP Loads, 2002-2007......................114

Figure 5-12: Comparison of Monthly OP Loads, 2002-2007...115

Figure 5-13: Comparison of NH_4-N Concentrations, 2002-2007...................................116

Figure 5-14: Seasonal Comparison of Baseflow and Storm NH_4-N Concentrations for Calibration (2002-2005) and Validation (2006-2007) Periods...............................118

Figure 5-15: Comparison of Ox-N Concentrations, 2002-2007.....................................119

Figure 5-16: Seasonal Comparison of Baseflow and Storm Ox-N Concentrations for Calibration (2002-2005) and Validation (2006-2007) Periods...............................120

Figure 5-17: Comparison of OP Concentrations, 2002-2007..121

Figure 5-18: Seasonal Comparison of Baseflow and Storm OP Concentrations for Calibration (2002-2005) and Validation (2006-2007) Periods...............................123

Figure 6-1: Location of Lake Manassas Watershed, Showing Major Streams, Stream Stations and Rain Gauges in the Occoquan Watershed..............................133

Figure 6-2: Lake Manassas Watershed Model Application Schema and Watershed Segmentation.........135

Figure 6-3: Segmentation of Lake Manassas Showing Selected Monitoring Stations....136

Figure 6-4: High and Low Tillage Cropland Distributions in Fauquier and Prince William Counties.........139

Figure 6-5: Comparison of Water Surface Elevation at Lake Manassas for Model Calibration (2002-2005) and Validation (2006-2007).........145

Figure 6-6: Comparison of Surface and Bottom Temperature at LM01 for Model Calibration (2002-2005) and Validation (2006-2007).........146

Figure 6-7: Comparison of Surface and Bottom DO Concentrations at LM01 for Model Calibration (2002-2005) and Validation (2006-07).........146

Figure 6-8: Comparison of Vertical Temperature Profile at LM01 near Lake Manassas Dam for the Calibration Period.........148

Figure 6-9: Comparison of Vertical DO Profile at LM01 near Lake Manassas Dam for the Calibration Period.........149

Figure 6-10: Comparison of Surface and Bottom OP Concentrations at LM01 for Model Calibration (2002-2005) and Validation (2006-07).........151

Figure 6-11: Comparison of Surface and Bottom NH_4-N Concentrations at LM01 for Model Calibration (2002-2005) and Validation (2006-2007).........151

Figure 6-12: Comparison of Surface and Bottom Ox-N Concentrations at LM01 for Model Calibration (2002-2005) and Validation (2006-2007).........152

Figure 6-13: Comparison of Chl *a* Concentrations at LM01 for Model Calibration (2002-2005) and Validation (2006-2007).........154

Figure 6-14: Seasonal OP Loads for Upper Broad Run Subbasin under Current and Pre-BMP Scenarios.........155

Figure 6-15: OP Yields in the Lake Manassas Drainage Areas under Current and Pre-BMP Scenarios.........156

Figure 6-16: Seasonal OP Concentration at LM01 under Current and Pre-BMP Scenarios.........157

Figure 6-17: Seasonal Chl *a* Concentration at LM01 under Current and Pre-BMP Scenarios 157

Figure 6-18: Comparison of Spatial Distribution of OP Concentrations along the Mainstem of Lake Manassas under Current and Pre-BMP Scenarios 158

Figure 6-19: Comparison of Spatial Distribution of Chl *a* Concentrations along the Mainstem of Lake Manassas under Current and Pre-BMP Scenarios 158

Figure 7-1: Location of Upper Broad Run Watershed, Showing Major Streams, Stream Stations and Rain Gauges in the Occoquan Watershed 167

Figure 7-2: The Upper Broad Run Watershed at the Coarser and Finer Segmentation ..171

Figure 7-3: Land Use Proportions in the Upper Broad Run Watershed in 1995, 2000 and 2006....172

Figure 7-4: Annual Precipitation Summary from 1993 to 2007 in the Upper Broad Run Watershed 177

Figure 7-5: Time Series Plots of Observed and Simulated Annual Flows 181

Figure 7-6: Scatter Plots of Observed and Simulated Monthly Flows 182

Figure 7-7: Time Series Plots of Observed and Simulated Annual Sediment Loadings .185

Figure 7-8: Scatter Plots of Observed and Simulated Monthly Sediment Loadings 185

List of Tables

Table 2-1: Summary of HSPF/AGCHEM Applications 11

Table 2-2: Application Summary of Linked Watershed and Receiving Water Quality Models 17

Table 3-1: Rainfall Summary (2002-2007) 37

Table 3-2: Annual Comparison by Variable and Year during Calibration and Validation Periods for the HSPF/PQUAL Application 39

Table 3-3: Seasonal Average Comparison by Variable during Calibration and Validation Periods for the HSPF/PQUAL Application 40

Table 3-4: Monthly R^2 by Variable during Calibration and Validation Periods for the HSPF/PQUAL Application 41

Table 3-5: Simulated Water Balance 41

Table 3-6: Simulated Nutrient Loss 41

Table 3-7: Meteorological Inputs and HSPF/PQUAL Parameters Included in the Sensitivity Analysis 43

Table 3-8: Sensitivity Index (*S*) of Average Annual Output Variables to HSPF/PQUAL Inputs and Parameters 44

Table 4-1: Soil Layer Depths for the AGCHEM Application in the Upper Broad Run Watershed 63

Table 4-2: Estimated Annual Nutrient Uptake Target for Crop Lands 67

Table 4-3: Estimated Monthly Fraction of Annual Nutrient Uptake for Crop Lands 67

Table 4-4: Estimated Soil Layer Fraction of Monthly Nitrogen and Phosphorus Uptake for Crop Lands 68

Table 4-5: Estimated Monthly Manure Nitrogen and Phosphorus Inputs to Pasture 70

Table 4-6: Estimated NH_4, NO_3 and PO_4 Inputs for Fertilized Land Uses (kg/ha) 73

Table 4-7: Annual Comparison by Variable and Year during Calibration and Validation Periods for the HSPF/AGCHEM Application 78

Table 4-8: Seasonal Average Comparison by Variable during Calibration and Validation Periods for the HSPF/AGCHEM Application 78

Table 4-9: Monthly R^2 by Variable during Calibration and Validation Periods for the HSPF/AGCHEM Application..79

Table 4-10: Simulated Nutrient Balance for Main Fertilized Land Types 80

Table 4-11: Meteorological Inputs, Nutrient Inputs and HSPF/AGCHEM Parameters Included in the Sensitivity Analysis 82

Table 4-12: Sensitivity Index (*S*) of Average Annual Output Variables to HSPF/AGCHEM Inputs and Parameters...83

Table 4-13: Sensitivity of Average Seasonal OP Loading to Fertilizer Application Time (as Percentage Change *SPD*) 85

Table 4-14: Sensitivity of Average Seasonal NH_4-N Loading to Fertilizer Application Time (as Percentage Change *SPD*)...87

Table 4-15: Sensitivity of Average Seasonal Ox-N Loading to Fertilizer Application Time (as Percentage Change *SPD*)...88

Table 5-1: List of Main PQUAL Parameters for Nitrogen and Phosphorus Simulation...99

Table 5-2: List of Main AGCHEM Parameters for Nitrogen Simulation 103

Table 5-3: List of Main AGCHEM Parameters for Phosphorus Simulation..................104

Table 5-4: Comparison of Annual Percent Differences (PD) of Nutrient (NH_4-N, Ox-N, OP) Loads, 2002-2007 111

Table 5-5: Comparison of Seasonal Average Percent Differences (PD) of Nutrient (NH_4-N, Ox-N, OP) Loads for Calibration and Validation Periods 111

Table 5-6: Comparison of Monthly R^2 of Nutrient (NH_4-N, Ox-N, OP) Loads for Calibration and Validation Periods..112

Table 5-7: Comparison of NH_4-N Baseflow and Storm Concentrations for Calibration and Validation Periods..117

Table 5-8: Comparison of Ox-N Baseflow and Storm Concentrations for Calibration and Validation Periods 117

Table 5-9: Comparison of OP Baseflow and Storm Concentrations for Calibration and Validation Periods 122

Table 6-1: Segment and Reach Characteristics of the Upper Broad Run and Middle Broad Run Subbasins 135

Table 6-2: Meteorological Inputs for the HSPF and CE-QUAL-W2 Models 138

Table 6-3: Differences between Nutrient Inputs for the Upper Broad Run and Middle Broad Run HSPF/AGCHEM Models 140

Table 6-4: Statistical Analysis of Summer Temperature and DO Concentrations at LM01 near Lake Manassas Dam 150

Table 6-5: Comparison between Simulated and Observed Nutrient (OP, NH_4-N and Ox-N) Concentrations at Lake Manassas Stations 153

Table 6-6: Average Annual Nutrient Loads for Upper Broad Run Subbasin under Current and Pre-BMP Scenarios 155

Table 6-7: Average Water Quality Concentrations at LM01 under Current and Pre-BMP Scenarios 156

Table 7-1: Segment and Reach Characteristics of the Upper Broad Run Watershed at the Coarser and Finer Segmentation 170

Table 7-2: Principal HSPF Calibration Parameters used in this Study 174

Table 7-3: Statistical Comparisons between Observed and Simulated Flows 181

Table 7-4: Statistical Comparisons between Observed and Simulated Sediment Loadings 184

Chapter 1. Introduction

1.1 Background and Motivation

Among the assessed 42% of total acres of lakes, reservoirs and ponds in the U.S., 45% are considered impaired (USEPA, 2002). Nutrients, primarily nitrogen and phosphorus, are found to be the most common pollutants affecting the impaired waters. Nutrient over-enrichment often triggers eutrophication, with negative environmental effects including algal blooms, increased turbidity and reduced oxygen concentration. The eutrophic waterbodies are poor drinking water sources and are undesirable for recreation and other beneficial water uses.

Nonpoint sources of nutrients, resulting from agricultural activities and urban development, have been identified as leading causes of the nutrient impairment (USEPA, 2002). One common approach to control the nonpoint sources of nutrients is by implementing nutrient management practices. It is important to characterize the nutrient sources and evaluate the nutrient management practices. However, due to their diffusive nature in the watershed, it can be difficult to characterize, non-point sources. A modeling approach has been increasingly used to help identify primary watershed processes and quantify the contributions from different loading sources. It also allows for a quick analysis of diverse nutrient management practice scenarios and provides best available data when direct measurements cannot be completed.

HSPF (Hydrological Simulation Procedure–Fortran) is one of the most extensively used watershed hydrology and water quality model for long–term continuous simulation in mixed agricultural and urban watersheds. With HSPF, nutrient processes in a watershed can be simulated by two modules: PQUAL or AGCHEM. Compared to the simpler empirical method PQUAL, AGCHEM may provide a better watershed nutrient simulation as a more detailed physical method by explicitly simulating complex nutrient transformations and transport in the soil. On the other hand, AGCHEM is more difficult to apply due to extensive data requirements, complicated module setup, and lack of modeling guidance. For a particular HSPF application, it is important to make a choice between using PQUAL or AGCHEM for effective nutrient simulation. However, it has not been well documented if AGCHEM can provide sufficiently more accurate nutrient modeling results than PQUAL, thus making the time and effort involved in applying HSPF/AGCHEM worthwhile for nutrient simulation in an agricultural and urbanizing watershed.

Extensive efforts have been spent on reviewing the applications of HSPF/AGCHEM, as shown in the next literature review chapter. The literature also indicates the need of a thorough sensitivity analysis to investigate significant inputs and parameters to better use the AGCHEM module for nutrient simulation. More attention could then be given to those inputs and parameters that are significant, based on sensitivity, during model development and calibration. By doing so, one can expect to save time and effort involved in applying HSPF/AGCHEM. The sensitivity analysis will also help with model uncertainty analysis and provide useful information for guiding AGCHEM usage.

Like other watershed models, HSPF provides a simple stream routing function to simulate flow and water quality transport and fate in reaches or streams. When the watershed nutrient management objective is water quality in lakes or reservoirs, such a watershed model cannot fully represent the complexities of nitrogen and phosphorus dynamics in the natural system. It is, therefore, becoming more and more popular to link watershed and receiving water quality models for effective nutrient simulation. The linked watershed-reservoir model approach can develop a direct cause-and-effect relationship between watershed nutrient management and downstream water quality in the receiving waterbody. However, it has not been tested if HSPF/AGCHEM can be well-applied within a linked watershed-reservoir system to evaluate nutrient management practices.

1.2 Research Goal and Objectives

The primary goal of this research is to investigate the AGCHEM module of HSPF for effectively simulating nutrient losses and nutrient management practices in agricultural and urbanizing watersheds. The study area is the Lake Manassas watershed, which includes one main waterbody, Lake Manassas, and its drainage areas in the Upper Broad Run and Middle Broad Run subbasins. Lake Manassas is nutrient enriched due to nutrient loads associated with agricultural activities and urban development in its drainage areas.

To achieve the goal, the following research objectives were investigated:

1. To investigate important inputs and parameters of HSPF/AGCHEM application for nutrient simulation in the Upper Broad Run subbasin.
2. To compare the AGCHEM and PQUAL modules of HSPF for nutrient simulation in the Upper Broad Run subbasin.
3. To apply HSPF/AGCHEM within a linked watershed-reservoir model system to evaluate nutrient management practice in the Lake Manassas watershed.

1.3 Dissertation Outline

This dissertation includes an introductory chapter, a literature review chapter, independent chapters in a technical paper format, a summary chapter, and a complete list of literature cited, followed by an appendix section.

Chapter 1: Introduction

This chapter describes background and motivation of the study, and discusses research goal and objectives.

Chapter 2: Literature Review

This chapter reviews literature related to watershed models, receiving water quality models and linked model applications for nutrient simulation. Methods of sensitivity analysis for the model applications are also included.

Chapter 3: Sensitivity Analysis, Calibration and Validation of a Watershed Model Application using HSPF with the Nutrient Algorithm PQUAL in Upper Broad Run Watershed, Virginia

This paper describes development, calibration and validation of the HSPF/PQUAL application in the Upper Broad Run watershed for simulating flow, sediment and nutrient transport and fate. "One-variable-at-a-time" sensitivity analysis was conducted on the calibrated HSPF/PQUAL model to investigate significant inputs and parameters with respect to flow, sediment and nutrient loadings. Three nutrient species involved in the model calibration, validation and sensitivity analysis were ammonium nitrogen (NH_4-N), oxidized nitrogen (Ox-N) and orthophosphate phosphorus (OP).

Chapter 4: Application and Sensitivity Analysis of a Watershed Model Application using HSPF with the Nutrient Algorithm AGCHEM in Upper Broad Run Watershed, Virginia

This paper describes development, calibration and validation of the HSPF/AGCHEM application in the Upper Broad Run watershed for nutrient simulation. "One-variable-at-a-time" sensitivity analysis was conducted to investigate significant inputs and parameters of the HSPF/AGCHEM application for nutrient load generation. Similar to Chapter 3, nutrient species involved in the model calibration, validation and sensitivity analysis were also ammonium nitrogen (NH_4-N), oxidized nitrogen (Ox-N) and orthophosphate phosphorus (OP).

Chapter 5: Comparison of two Nutrient Simulation Algorithms of HSPF in Upper Broad Run Watershed, Virginia

This paper compares the AGCHEM and PQUAL modules of HSPF for nutrient simulation in the Upper Broad Run watershed. The comparison was mainly based on the model performances for simulating nutrient (NH_4-N/Ox-N/OP) loadings from the watershed and in-stream nutrient (NH_4-N/Ox-N/OP) concentrations.

Chapter 6: Evaluation of Nutrient Management Plans Using a Linked Watershed-Reservoir Model

This paper demonstrates application of HSPF/AGCHEM within a linked watershed-reservoir model system in the Lake Manassas watershed. In this linked model application, the Lake Manassas CE-QUAL-W2 model was calibrated by using the outputs from the HSPF/AGCHEM models of the Upper Broad Run and Middle Broad Run subbasins. The calibrated model system was then used to investigate water quality impacts by implementing nutrient management plan in the watershed.

Chapter 7: Evaluating HSPF Performance of Flow and Sediment Prediction at Multiple Watershed Segmentations in Upper Broad Run Watershed, Virginia

This paper evaluates how well HSPF performs with respect to flow and sediment prediction at multiple watershed segmentation levels in the Upper Broad Run watershed. In the evaluation, the coarser and finer segmented HSPF model applications were used as a prediction tool when extended approximately 10 years outside their calibration period under varying meteorology and land use conditions. Although it is not directly related to the research objectives, findings from this paper are expected to help practitioners to obtain better guidance and more confidence in using the model as a prediction tool.

Chapter 8: Conclusions and Recommendations

This chapter provides a summary of research results and reviews whether the objectives have been achieved. Recommendations for future research and modeling improvement are also included.

References Cited: This section provides a complete list of literature references cited.

Appendix: This section describes detailed development of nutrient inputs for the HSPF/AGCHEM applications in the Lake Manassas watershed.

Chapter 2. Literature Review

This chapter provides a review of model applications for nutrient simulation as well as for sensitivity analysis methods. The commonly-used surface water quality models are generally categorized into watershed models and receiving water quality models. Some linked watershed and receiving water quality model applications are also discussed. Most efforts were spent on reviewing the applications related to the HSPF watershed model.

2.1 Watershed Models

The intent of watershed models, sometimes called rainfall-runoff models or nonpoint source models, is to simulate various hydrological processes and/or associated water quality components in a watershed. Some of the commonly used watershed models include: AGNPS (Agricultural Nonpoint Source Pollution Model) (Young et al., 1994), HSPF (Hydrologic Simulation Program-FORTRAN) (Bicknell et al., 2005), ANSWERS (Areal Nonpoint Source Watershed Environment Response Simulation) (Beasley et al., 1980), SWMM (Storm Water Management Model) (Huber et al., 1988) and SWAT (Soil and Water Assessment Tool) (Neitsch et al., 2002).

According to the degree of spatial variability, watershed models can be classified as distributed-parameter or lumped-parameter models. Distributed-parameter models divide the watershed into smaller cells with computation units that have homogeneous characteristics. The spatial variability of the watershed can be easily represented. AGNPS and ANSWERS are typical distributed-parameter models. However, distributed-parameter models can be computationally intensive with a significantly large number of input parameters. Lumped-parameter models consider the watershed or a portion of it as one unit and the watershed parameters are averaged over the unit. Such models cannot detect the spatial variability within each computation unit. However, the spatial variability of the watershed can be addressed with these models by reducing the computational unit areas. HSPF, SWAT and SWMM are such lumped-parameter models.

Based on the temporal scale, watershed models can be classified as either event-oriented or continuous models. Event-oriented models, such as AGNPS and ANSWERS, simulate the response of a watershed to major storms. Continuous models simulate all the processes on a time interval like a day or an hour, thus allowing a continuous balance of water and pollutant mass in the system and providing a long time-series of water and pollutant loadings. HSPF and SWAT are typical continuous models. SWMM has both continuous and storm event simulation capabilities. For long-term watershed management studies, continuous models are more useful (Borah, 2002). Additional efforts are always required when event-oriented models are applied for these studies. Mostaghimi et al. (1997) used AGNPS to evaluate management alternatives in the Owl Run watershed, a small agricultural watershed located in Fauquier County, Virginia. To allow the model to be used for the evaluation, a very complex annualization procedure was developed to convert the single-event simulation results to annual average values. Realizing the limitation, AGNPS was modified into AnnAGNPS (Annualized Agricultural Nonpoint Source Model) to expand its application to continuous multi-event systems (Bingner and Theurer, 2001). Similarly, ANSWERS-2000 emerged from ANSWERS as a continuous model (Bouraoui and Dillaha, 1996; Bouraoui et al., 2002).

For nutrient simulation, watershed models concentrate on the generation of nutrients and their transport across the land surface to waterways and/or through the soil profile to ground water. Nutrient transport and fate can be represented at various levels of detail, from simple empirical relationships to physically-based approaches. Generally, the simple empirical relationships estimate nitrogen and phosphorus yield as a function of nutrient concentration, runoff volume and sediment yield. Nutrient transformations are not considered in the watershed models, such as SWMM, AGNPS and ANSWERS, based on the simple empirical relationships. The physically-based approaches are generally used for nutrient simulation in the continuous watershed models, including AnnAGNPS, ANSWERS-2000, and SWAT. HSPF has nutrient simulation capabilities based on both empirical relationships and the physically-based approach.

Among the continuous watershed models, SWAT is promising for hydrologic and nutrient simulation in predominantly agricultural watersheds (Borah and Bera, 2003; Borah and Bera, 2004). Vache et al. (2002) applied SWAT to predict nitrate loads from the Walnut Creek watershed in Iowa and reported reasonable simulation results. SWAT was found to predict organic N and P yields well from the Bosque River watershed (Santhi et al., 2001). Nutrient transformations and interactions in soil layers were simulated in the SWAT applications, including plant uptake of nutrients and the mineralization of organic nutrients in plant residue. The fundamental nutrient simulation mechanisms behind AnnAGNPS and ANSWERS-2000 are similar to those of SWAT. AnnAGNPS was mostly applied to relatively small agricultural watersheds to predict runoff, sediment and nutrient losses (for example, Suttles et al., 2003; Baginska et al., 2003; Yuan et al., 2011). ANSWERS-2000 was tested on two small agricultural watersheds in Georgia and on a large agricultural watershed in Virginia (Bouraoui and Dillaha, 2000). The test results indicated the model performed reasonable well in predicting runoff, sediment, nitrate, ammonium, sediment-bound TKN, and orthophosphate phosphorus losses.

For watersheds comprised of mixed land uses, HSPF is the most extensively used hydrologic and nonpoint source pollution model (Borah and Bera, 2004). Borah and Bera (2003) critically reviewed mathematical bases of HSPF and another ten watershed models and recognized HSPF’s strengths for continuous simulations in mixed agricultural and urban watersheds. The following literature view focuses on describing HSPF and its applications.

HSPF is a comprehensive lumped-parameter model for simulating hydrologic and associated water quality processes in a watershed. It originated from the Stanford Watershed Model (SWM) developed in 1966. SWM was further improved and resulted in Hydrocomp Simulation Program (HSP) in 1969. In the 1970s, HSFP experienced continual modification and incorporated the watershed scale Agricultural Runoff Model (ARM) and urban Nonpoint Simulator (NPS). All essential functions of HSP, ARM and NPS were the basis of HSPF. The model has been continuously updated and the latest version is HSPF 12.2 (Bicknell et al, 2005). It is now incorporated into the Better Assessment Science Integrating Point and Nonpoint Sources (BASINS) package developed for EPA and widely used to support watershed and water quality studies.

HSPF describes a continuous series of hydrological events by using intensive rainfall and other meteorological data, such as temperature, solar radiation, wind speed, potential evapotranspiration, and cloud cover (Xu, 2005). Pervious and impervious land types were defined based on hydrological characteristics. On pervious lands, infiltration is considered and water movement is modeled along overland flows, interflow and baseflow with theoretical and empirical equations. Water quality constituents can be simulated in a simple way (PQUAL) or a detailed agricultural chemical approach (AGCHEM). PQUAL simulates water quality constituents by assuming a simple relationship with water and sediment yield. It originates from the NPS and is typically used for urban areas. AGCHEM originates from ARM and provides a detailed simulation of the dynamic and continuous processes that affect the storages and outflow of nutrients from fertilized fields. On impervious lands, no infiltration is considered and water quality constituents are simulated using the simple empirical relationship with water and sediment yield.

There have been many hundreds of applications of HSPF in different geographic regions all over the world (for example, Imhoff et al.,2010; Diaz-Ramirez et al., 2008; Mishra et al., 2007; Hayashi et al., 2001). Most of the applications focus on hydrological modeling. Bergman et al. (2002) have observed that HSPF is increasingly used for water quality assessment studies involving sediment, nitrogen and phosphorus. Numerous HSPF applications for nutrient simulation have been reported in literature (for example, Chun et al., 2001; Rahman and Salbe, 1995; Tsihrintzis et al., 1996). One of the largest applications of HSPF is in the 64,000 square mile Chesapeake Bay watershed. The USEPA’s Chesapeake Bay Program uses HSPF to simulate watershed loadings of flow, sediment and nutrients to the tidal regions of the Bay (Donigian et al., 1994). It is also used to evaluate water quality effects of nutrient and sediment reduction plans (Cerco et al., 2002).

As mentioned earlier, HSPF provides two nutrient simulation algorithms: PQUAL and AGCHEM. Of the two algorithms, PQUAL is easier to apply and generally used in watershed nutrient simulation (for example, Bergman et al., 2002; El-Kaddah and Carey, 2004). Xu (2005) used the PQUAL module for nutrient simulation in six HSPF applications in the Occoquan watershed. These HSPF/PQUAL applications simulate nutrient transport and fate well except in the Cedar Run subbasin, which is an agricultural intensive area. The study found a general under-prediction of nitrate loads in the Cedar Run subbasin and pointed out a possible reason for this being the lack of simulation of manure and fertilizer application. HSPF/AGCHEM has also been applied to simulate nutrient processes in several studies. Table 2-1 summarizes some of the HSPF/AGCHEM applications found in the literature.

Table 2-1: Summary of HSPF/AGCHEM Applications

Location	Watershed characteristics	Modeled constituents	Model applications and conclusions	Reference
Wolf River watershed, Mississippi	A 379.69 mi^2 undeveloped watershed	NO_3, NH_3, and PO_4	To evaluate impacts of fertilization on the in-stream nutrient simulation. Nutrient input estimates based on current or historical fertilization practices were found to generate quite different nutrient loadings, which then had strong impacts on the in-stream nutrient concentrations.	Liu et al., 2005
Upper North Bosque River watershed, Texas	A 355.6 mi^2 rural watershed with primary land use of rangeland and forage field	Streamflow, TSS, NO_3, organic N, PO_4, and particulate P	To evaluate HSPF/AGCHEM and SWAT for simulating flow, sediment and nutrient loadings. Both models provided reasonable predictions of average daily flow and TSS loadings, while SWAT performed better than HSPF for nutrient simulation.	Saleh and Du, 2004
Ipswich River watershed, Massachusetts	A 155.99 mi^2 urbanized watershed with 32% of urban area	Streamflow, NO_3, and NH_3	To predict the impacts of land use on stream water quality. It was found that urbanization could result in large increase of nutrient concentration in the stream.	Filoso et al., 2004
Iowa River basin, Iowa	A 2795.38 mi^2 agricultural watershed with 45% of corn and 22% of soybean cropland	Streamflow, sediment, alachlor, NO_3, and NH_3	To demonstrate the application of HSPF/AGCHEM in a large watershed. Flow prediction ranged from fair to good without snow simulation. Poor to fair performance of sediment and nutrient simulation was attributed to model deficiencies in flow simulation, insufficient calibration, and lack of data.	Bicknell et al., 1984
A small west Tennessee watershed	A 0.07 mi^2 agricultural watershed with 100% corn cropland	Flow, sediment, atrazine, NO_3, NH_3, and TKN	To demonstrate the application of HSPF/AGCHEM in a small watershed. The monthly simulation of hydrology and sediment were generally good, while simulated monthly NO_3, NH_3 were fair.	Moore et al., 1988

Most of the HSPF/AGCHEM applications focused on how to set up the AGCHEM module. As indicated by Kieffer (2002), the complicated module structure is just one of the reasons that limit the AGCHEM applications to nutrient modeling. Some other reasons also prevent the AGCHEM module from being effectively used, including extensive data requirements and lack of documentation. Realizing the importance of reliable data inputs for modeling, Liu et al. (2005) investigated how to develop nutrient inputs based on historical fertilization practices for long term simulations.

Several studies attempted to compare the AGCHEM module with other nutrient simulation models and approaches. Im et al. (2003) compared HSPF/AGCHEM and SWAT for simulating stream flow, sediment and nutrient loadings from the Polecat Creek watershed, a urbanizing watershed in Virginia. In the study, HSPF provided a better flow simulation. Simulated annual and monthly TKN and TP loads by HSPF/AGCHEM were also closer to observed values than those simulated by SWAT. Saleh and Du (2004) compared HSPF/AGCHEM and SWAT for simulating flow, sediment and nutrient loadings from the Upper North Bosque River watershed, a rural watershed highly impacted by dairy operations in Central Texas. Both models provided reasonable predictions of average daily flow and TSS loadings. SWAT was generally a better predictor of daily and monthly nutrient loadings, probably due to ease of field management practices input (fertilizer and manure application) in the SWAT model. Liu et al. (2008) conducted comparison analysis of PQUAL and AGCHEM for simulating in-stream nutrient concentrations in the Wolf River watershed. In the study, AGCHEM was only applied in a small percentage (12.4%) of the total area and the inclusion of AGCHEM module didn’t significantly improve model performance.

More studies are needed to explore the aspects of effectively using HSPF/AGCHEM for nutrient simulation. More specifically, it is important to know significant inputs and parameters for the model application. Without knowing the significant facts, one may waste tremendous amounts of time and resources during model development and calibration. In addition, further comparison studies between PQUAL and AGCHEM should be conducted in an agricultural and urbanizing watershed. Since AGCHEM application normally involves more time and effort, it is better for the application to provide more accurate nutrient modeling results than PQUAL.

2.2 Receiving Water Quality Models

Receiving water quality models concentrate their efforts on hydrodynamics and water quality processes in receiving waterbodies, such as rivers, lakes, reservoirs and estuaries. The spatial and temporal characteristics of the receiving waterbodies can be described in the models with varying complexity, ranging from simple steady-state 1-D models such as QUAL2E to complex 3-D models such as WASP (Water Quality Analysis Simulation Program) software package.

QUAL2E is a steady-state one-dimensional water quality model that simulates nutrient dynamics, algal production and DO interactions. It is suitable for modeling streams and rivers, which are assumed to be trapezoidal and divided into homogeneous reaches. The governing equations describing the reaches are advection-dispersion-reaction equations. A finite difference scheme is applied to solve the governing equations. Typical applications of QUAL2E include stream assimilative capacity, waste load allocation studies and diurnal response to climatology (Brown and Barnwell, 1987). QUAL2E has been incorporated as an in-stream water quality model into the BASINS package.

The WASP software package is a USEPA generalized modeling framework, which is detailed and fully dynamic with 1-D, 2-D or 3-D spatially simulation capabilities. The current WASP software package consists of two computer programs, DYNHYD and WASP. DYNHYD is a hydrodynamics program capable of simulating water velocities, water heads, flows and volumes. WASP is a water quality program that can simulate the transport and fate of conventional and toxic contaminants in water columns as well as benthic layers (Wool et al., 2003). The WASP program includes two scientific modules to simulate water quality processes: EUTRO for conventional contaminants and TOXI for toxic contaminants. Most WASP applications are for EUTRO. EUTRO is capable of modeling eight water quality variables (i.e., DO, CBOD, phytoplankton, chlorophyll *a*, ammonia, nitrate, organic nitrogen, and orthophosphate) in the water columns and benthic layers.

CE-QUAL-W2 is a two-dimensional hydrodynamic and water quality model that provides a detailed description of algae/nutrient/DO dynamics in relatively long and narrow waterbodies such as rivers, lakes and reservoirs (Cole and Wells, 2008). It assumes homogeneity in the lateral direction and describes the longitudinal and vertical variations of flow and water quality characteristics. The fundamental mechanisms of the model are the conservation of mass, energy and momentum. In CE-QUAL-W2, waterbodies are defined by a series of control volumes with horizontal layers in the vertical direction of each longitudinal segment (Xu et al., 2006). The governing equations describing the control volumes include the continuity equation, momentum equations for the x- and z-axis, the free surface equation, the state equation, and the hydrostatic pressure equation. These equations are solved by using a finite difference method with a variety of user-selectable numerical schemes. The model is able to simulate water surface elevations, velocities, temperatures, as well as 21 other water quality constituents, such as DO, carbonaceous biochemical oxygen demand (CBOD), ammonium, nitrate+nitrite, orthophosphate phosphorus, algae, etc.

CE-QUAL-W2 has been successfully applied to more than 1000 waterbodies worldwide and the example applications can be found in Cole and Wells (2008). The CE-QUAL-W2 application for the Occoquan Reservoir can be traced back to 1994. According to NVPDC (1994), CE-QUAL-W2 was used to 1) simulate the seasonal stratification; 2) to simulate longitudinal variations; 3) to represent the variable layer heights; and 4) to evaluate water quality control and management.

There are other receiving water quality models, such as AQUATOX (USEPA, 2004) and BATHTUB (Walker, 1986). In addition, some of the watershed models also provide simple in-stream routing to simulate the processes that occur in one dimensional, completely mixed waterbody. For example, the RCHRES module of HSPF use a storage-volume relationship defined in FTABLEs to simulate hydraulic behavior in the streams. Diverse water quality constituents, including DO, CBOD, nitrogen, phosphorus, algae and phytoplankton, can be simulated under the RCHRES module.

2.3 Linked Watershed and Receiving Water Quality Model Applications

Recently, integrated watershed management is becoming more and more popular for water quality protection. This requires a model with capabilities of simulating both watershed processes and resulting water quality impacts in a waterbody. Many watershed models, like HSPF and SWAT, have some limited capabilities in this area. With HSPF, runoff and associated water quality constituents from pervious and impervious lands, both in surface and subsurface components, along with point source contributions, drains to channel reaches. However, HSPF assumes the reaches to be completely mixed and unidirectional, which sometimes cannot provide a sufficient description of the physical characteristics as well as associated processes. For example, although HSPF considers nutrient transformations in reaches, it cannot fully represent the spatial distribution of nitrogen and phosphorus due to phytoplankton accumulation in the epilimnion and oxygen depletion in the hypolimnion.

Such limitation is more apparent when a watershed drains into larger waterbodies such as lakes, reservoirs and estuaries. Generally, 2-D or 3-D computations are required in the larger waterbodies, where stratification and mixing mechanisms are of concern. To overcome the limitation, one approach is to represent the complex waterbodies with appropriate receiving water quality models and then link them to the watershed model. The linked modeling framework coupling watershed model and receiving water quality model would represent the complex system more accurately and flexibly. Within the linked modeling framework, the watershed model estimates loadings of water and pollutants into a waterbody, while the receiving water quality model analyzes resulting water quality impacts in the waterbody in response to the loadings from its contributing watershed.

Many studies have attempted to link watershed and receiving water quality models. Table 2-2 summarizes some applications linking commonly-used watershed and receiving water quality models. A good example of the linked model applications is the Occoquan model. The first completed linked Occoquan model was for the 1988-1992 period and it was then updated for the 1993-1997 period, including six applications of HSPF and two applications of CE-QUAL-W2 which were linked in a complex way to represent the characteristics of the Occoquan watershed (Xu, 2005; Xu et al., 2007). The Occoquan model is updated in five-year increments and the latest update was for the 2002-2007 period. During the latest update, a finer segmentation was performed on the Occoquan watershed that resulted in seven applications of HSPF. In the linked Occoquan model, the HSPF applications simulate watershed loadings of flow, sediment and nutrients into two main waterbodies including Lake Manassas and Occoquan Reservoir. Both waterbodies are simulated with CE-QUAL-W2 to provide a detailed computation of hydrodynamic and algae/nutrient/DO dynamics.

In addition to a better representation of the natural system, the Occoquan model develops a direct linkage between upland activities and downstream water quality. Xu (2005) applied the Occoquan model to evaluate the impact of land use changes on water quality. The model is also expected to be used to investigate the responses of receiving water quality to watershed management plans. For this, the HSPF applications in the Occoquan model are proposed to include a more detailed nutrient simulation algorithm (AGCHEM) with capabilities to represent these plans.

Table 2-2: Application Summary of Linked Watershed and Receiving Water Quality Models

Location	Models	Applications	Reference
Lake Gaston, Virginia	SWMM→QUAL2E	To examine in-lake water quality response to upstream water withdrawal.	Gatling et al., 2000
Occoquan Watershed, Virginia	HSPF→CE-QUAL-W2	To evaluate the impacts of land use changes on water quality.	Xu, 2005
Chesapeake Bay	RADM*→HSPF→CE-QUAL-ICM**	To determine the pollutant contributions from multi-state sources and evaluate BMP implementation level to mitigate pollution stress. Types of BMPs simulated include structural and non-structural urban and agricultural practices	CBPO, 2004
Swift Creek Reservoir watershed, Virginia	HSPF→CE-QUAL-W2	To develop a water-quality-based structural urban BMP design approach.	Wu, 2004
Lake Waco-Bosque River watershed, Texas	SWAT→CE-QUAL-W2	To evaluate the impacts of dairy BMPs and WWTP phosphorus control strategies on lake water quality.	Flowers et al., 2001
Cedar Creek watershed, Texas	SWAT→CE-QUAL-W2	To simulate the combined processes of water quantity and quality both in the upland watershed and downstream waterbody.	Debele et al., 2006
Lake Thonotosassa watershed, Florida	SWMM→WASP	To simulate water quantity and quality for the entire system.	Dames and Moore, 1992

* RADM stands for Regional Acid Deposition Model
** ICM stands for Integrated Compartment Model

2.4 Sensitivity Analysis Methods

Sensitivity analysis characterizes the impact of changes in model inputs on the model outputs (Tang et al., 2007). It is often used to identify critical parameters and inputs, which indicate where most time and effort should be spent in the parameter estimation process.

There are many techniques for conducting sensitivity analysis (SA), such as the nominal range sensitivity method (also called "one-variable-at-a-time" sensitivity analysis), Morris method and generalized sensitivity analysis (GSA, also called regionalized sensitivity analysis), analysis of variance (ANOVA), Sobol's method and Fourier amplitude sensitivity test (FAST). Generally, the techniques can be categorized into two main groups: local method and global method. Local methods evaluate the impact of a parameter at a certain point (default or calibrated value) on the model output (Griensven et al., 2006). “One-variable-at-a-time” sensitivity analysis is a typical local method. Alternatively, global methods (Morris method, GSA, ANOVA, Sobol’s method and FAST) attempt to explore the full parameter space.

All the methods have their advantages and limitations. Generally, local methods have the advantages of being easy to implement with low computational cost. However, there are some limitations in using local methods, including: 1) lack of consideration of model nonlinearity and parameter interactions; and, 2) lack of consideration of different degrees of uncertainty associated with each parameter (White and Chaubey, 2005). Therefore, one needs to be careful when interpreting the SA results when a local method is applied to any model with strong nonlinearity. On the other hand, global methods can provide relatively more robust and reliable SA results, although the computational cost is often very high for complex models.

A few researchers have applied global SA methods in water quality modeling up to a medium level of complexity (Lence and Takyi, 1992; Adams, 1998). Zheng and Keller (2006) applied GSA to WARMF (Watershed Analysis Risk Management Framework) to understand parameter sensitivity and its management implications. For simplicity, the SA was carried out for a single “representative” catchment in the study. The study estimated that it took about10,000 model runs to finally identify sensitive parameters. Tang et al. (2007) tested three global methods including GSA, ANOVA and Sobol’s method on the lumped Sacramento soil moisture accounting model (SAC-SMA) coupled with SNOW-17. It was found that all the three global methods need too many samples to cover the full parameter ranges. Therefore, the inefficiency resulting from the need for a large number of simulations prevents the global methods from being widely used.

Currently, performing a SA for complex watershed models remains a challenge. Over-parameterization is very common for these models. The importance of computational efficiency is apparent when considering the over-parameterization and complex nature of the watershed models, which may have in excess of 100 parameters in varying ranges (Ravalico, 2005). Additionally, multiple model output variables (e.g., flow, sediment, nitrogen and phosphorus) have to be considered while conducting SA for these models (Griensven et al., 2006). Therefore, SA methods are needed that can accommodate a large number of parameters while considering several output variables. “One-variable-at-a-time” sensitivity analysis is the most common choice for conducting SA for the complex watershed models (Zheng and Keller, 2006). Although this local method has its limitations, so far it better meets the demands of sensitivity analysis studies than other methods.

Most studies with the “one-variable-at-a-time” sensitivity analysis provided SA results as individual sensitivity indices (usually expressed in a normalized form), which are defined as the change in each model output variable in response to change in a single parameter (Shoemaker and Benaman, 2003). The individual sensitivity indices are then ranked to determine the sensitive parameters for various model output variables (Lenhart et al., 2002; Wu, 2004). Lenhart et al. (2002) applied two approaches (both are nominal range sensitivity methods with different ways of defining parameter variation, Δx) to study the parameter sensitivity of SWAT with respect to seven output variables (surface runoff, evapotranspiration, sediment yield, nitrate, organic N, total phosphorous and organic P). In the first approach, the parameter variation Δx was 10% of the initial value of the parameter. In the second approach, the parameter variation Δx was 25% of the mean value of the parameter. Both approaches in the study provided similar sensitivity results. For a standard sensitivity analysis, using a 10% variation is considered to be arbitrary but adequate (Fontaine and Jacomino, 1997).

A large amount of effort was spent on reviewing sensitivity analysis studies for HSPF, the most comprehensive watershed model. Only a few studies have been reported in the literature and these studies were all based on the “One-variable-at-a-time” sensitivity analysis. Fontaine and Jacomino (1997) performed SA on HSPF application for a 6.2 mi^2 catchment in eastern Tennessee to identify sensitive parameters with respect to streamflow, flux of sediment and Cs^{137}. The sensitivity analysis results illustrated that the accuracy of simulated flux of sediment and Cs^{137} depended on accurate streamflow simulation. Donigian and Love (2007) performed SA on HSPF application in the Housatonic River watershed to identify sensitive parameters for streamflow, TSS (total suspended solid) loading and water temperature. Besides model parameters, meteorological inputs (i.e., precipitation, air temperature and solar radiation) were also included in the sensitivity analysis. The meteorological inputs (especially precipitation) were subject of investigation because they were considered to be the primary sources of uncertainty under wet weather conditions, which might greatly impact streamflow simulation. One preliminary sensitivity analysis was performed on meteorological inputs and HSPF/AGCHEM parameters with respect to nutrient (NO_3, NH_4 and PO_4) loadings in the Swift Creek Reservoir watershed (Wu, 2004). Non-point sources of nutrients in the watershed originated from fertilizer and manure applied on agricultural and residential areas. The study didn't include the fertilizer and manure inputs in the sensitivity analysis and a more thorough sensitivity analysis involving these inputs was suggested for future research.

2.5 References

Adams, B. V.,1998. Parameter Distributions for Uncertainty Propagation in Water Quality Modeling. PhD. Dissertation, Duke University.

Baginska, B., Milne-Home, W., and Cornish, P.S., 2003. Modeling nutrient transport in Currency Creek, NSW with AnnAGNPS and PEST. Environ. Model. Software. 2003, 18, 801-808.

Beasley, D. B., Huggins, L.F., and Monke, E.J.,1980. ANSWERS: A Model for Watershed Planning. Transactions of the ASAE, 23(4), 938-944.

Bergman, M.J., Green, W., and Donnangelo, L.J., 2002. Calibration of storm loads in the south Prong watershed, Florida, using BASINS/HSPF. Journal of the American water resources association. 38(5): 1423-1236.

Bicknell, B.R., Donigian, A.S., and Barnell, T.A.,1984. Modeling Water Quality and the Effects of Agricultural Best Management Practices in the Iowa River Basin. Journal of Water Science and Technology. 17: 1141-1153.

Bicknell, B.R., Imhoff, J.C., Kittle, J.L., Jobes, T.H., and Donigian, A.S, 2005. Hydrological Simulation Program -Fortran (HSPF). User's manual for release 12.2. U.S.EPA. National Exposure Research Laboratory, Athens, GA.

Bingner, R. L., and Theurer. F. D., 2001. AnnAGNPS Technical Processes: Documentation Version 2. Available at www.sedlab.olemiss.edu/AGNPS.html. Accessed 26 July, 2010.

Borah, D.K., 2002. Watershed Scale Nonpoint Source Pollution Models: Mathematical bases. 2002 ASAE International Meeting/CIGR World Congress, Chicago, IL. Paper no. 022091.

Borah, D. K., and Bera, M., 2003. Watershed-scale hydrologic and nonpoint-source pollution models: Review of mathematical bases. Trans. ASAE 46(6): 1553-1566.

Borah, D. K., and Bera, M., 2004. Watershed-scale hydrologic and nonpoint-source pollution models: Review of applications. Trans. ASAE 47(3): 789-803.

Bouraoui, F., and Dillaha, T. A.,1996. ANSWERS-2000: Runoff and sediment transport model. J. Environ. Eng. 122(6):493-502.

Bouraoui, F., and Dillaha, T. A., 2000. Answers-2000: Nonpoint source nutrient planning model. J. Environ. Eng. 126: 1045-1055.

Bouraoui, F., Braud, I., and Dillaha, T. A., 2002. ANSWERS: A nonpoint-source pollution model for water, sediment, and nutrient losses. Chapter 22 in Mathematical Models of Small Watershed Hydrology and Applications, 833-882.

Brown, L. C., and Barnwell, T. O., 1987. The Enhanced Stream Water Quality Models QUAL2E and QUAL2E-UNCAS: Documentation and User Manual. Environmental Resources Laboratory, Environmental Protection Agency, Athens, Georgia.

Cerco, C.F., Linker, L., Sweeney, J., Shenk, G., and Butt, A.J., 2002. Nutrient and Solid Controls in Virginia’s Chesapeake Bay Tributaries. Journal of Water Resources Planning and Management, 128(3): 179-189.

Chesapeake Bay Program Office (CBPO), 2004. Tributary Strategy Tool. Available at http://www.chesapeakebay.net/tribtools.htm. Accessed 30 July, 2007.

Chun, K.C., Chang, R.W., Williams, G.P., Chang, Y.S., Tomasko, D., LaGoory, K., Ditmars, J., Chun, H.D., and Lee, B.K., 2001. Water quality issues in the Nakdong River basin in the Republic of Korea. Environmental Engineering and Policy. 2(3): 131-143.

Cole, T. M., and Wells, S. A., 2008. CE-QUAL-W2: A Two-Dimensional, Laterally Averaged, Hydrodynamic and Water Quality Model, Version 3.6 User Manual. In. Washington, DC: U.S. Army Corps of Engineers.

Debele, B., Srinivasan R., and Parlange. J. Y., 2006. Coupling upland watershed and downstream waterbody hydrodynamic and water quality models (SWAT and CE-QUAL-W2) for better water resources management in complex river basins. Environ Model Assess.

Diaz-Ramirez, J.N., Perez-Alegria,v, and McAnally, W.H., 2008. Hydrology and Sediment Modeling Using HSPF/BASINS in a Tropical Island Watershed. Transactions of the ASABE 51(5):1555-1565.

Donigian, A. S., Bicknell, B. R., Patwardham, A. S., Linker, L. C., and Chang, C., 1994. Chesapeake Bay Program: watershed model application to calculate bay nutrient loadings. U.S. EPA-903-R-94-042, Chesapeake Bay Program Office. U.S.EPA. Annapolis, Maryland.

Donigian, A.S., and Love, J.T., 2007. The Housatonic River Watershed Model: Model Application and Sensitivity/Uncertainty Analysis. 7th International IWA Symposium on System Analysis and Integrated Assessment in Water Management, May 7-9, 2007. Washington, DC.

El-Kaddah, D.N., and Carey, A.E., 2004. Water quality modeling of the Cahaba River, Alabama. Environmental Geology. 45: 323-338.

Filoso, S., Vallino, J., Hopkinson, C., Rastetter, E., and Claessens, L., 2004. Modeling Nitrogen Transport in the Ipswich River Basin, Massachusetts, using a Hydrological Simulation Program Fortran (HSPF). Journal of the American Water Resources Association 40 (5): 1365–1384.

Flowers, J. D., Hauck, L. M., and Kiesling, R., 2001. USDA: Lake Waco-Bosque River Initiative: Water Quality Modeling of Lake Waco Using CE-QUAL-W2 for Assessment of Phosphorus Control Strategies. Texas.

Fontaine, T. A., and Jacomino, V. M. F, 1997. Sensitivity analysis of simulated contaminated sediment transport. JAWRA 33: 313-326.

Gatling, L. A., Kardash, A. O., and Yoon, J., 2000. Spatiotemporal Water Quality Modeling of Pipeline Water Intake Lake Gaston, Virginia. Paper presented at the Building Partnerships - 2000 Joint Conference on Water Resource Engineering and Water Resources Planning and Management, Virginia.

Griensven, A.V., Meixner, T., Grunwald, S., Bishop, T., Diluzio, M., and Srinivasan, R., 2006. A global sensitivity analysis tool for the parameters of multi-variable catchment models. Journal of Hydrology, 324: 10–23.

Hayashi, S., Murakami, S., Watanabe, M., and Xu, B., 2001. HSPF simulation of runoff and sediment loads in the upper Changjiang River Basin, China. Journal of Environmental Engineering 130(7), 801–815.

Huber, W. C., and Dickinson, R. E.,1988. Storm Water Management Model User's Manual, Version 4. Athens, Georgia, Environmental Protection Agency.

Im, S., Brannan, K.M., and Mostaghimi, S., 2003. Simulating Hydrology and Water Quality Impacts in an Urbanizing Watershed. JAWRA 39(6): 1465-1479.

Imhoff, J.C., Kittle, J.L., Gonzales, B.B., Donigian, A.S., Deliman, P.N., Elliot, W.J., and Flanagan, D.C., 2010. Development and Demonstration of a Hybrid Modeling Capability within the Fort Benning HSPF Watershed Model: Refinement of Unpaved Road Simulation Using

WEPP:Road. Proceedings of AWRA 2010 Spring Specialty Conference. March 29-31, 2010. Orlando, FL.

Kieffer, J.M., 2002. Development of a nutrient and dissolved oxygen water quality model for the Saint Louis Bay watershed. M.S. thesis, Mississippi State University.

Lence, B. J., and Takyi, A. K.,1992. Data Requirements for seasonal discharge programs: An Application of a Regionalized Sensitivity Analysis. Water Resources Research. 28 (7): 1781-1789.

Lenhart, T., Eckhardt, K., Fohrer, N., and Frede, H. G., 2002. Comparison of two different approaches of sensitivity analysis. Phys. Chem. Earth, 27(9-10), 645-654.

Liu, Z., Kieffer, J. M., Hashim, N.B., Kingery, W.L., and Huddleston, D.H., 2005. The Influence of Crop Fertilization Practices on Nutrient Input Parameters for Water Quality Modeling in the Wolf River Watershed Using HSPF. International Journal of Civil and Environmental Engineering. 1(1): 1-17.

Liu, Z., Kingery, W.L., Huddleston, D. H., Hossain, F., Hashim N. B., and Kieffer J. M., 2008. Application and evaluation of two nutrient algorithms of Hydrological Simulation Program Fortran in Wolf River watershed. Journal of Environmental Science and Health, Part A 43(7):738-48.

Mishra, A., Kar.S, and Singh, V. P., 2007. Determination of runoff and sediment yield from a small watershed in subhumid subtropics using the HSPF model. Hydrological Processes, 21 (22): 3035-3045.

Moore, L.W., Matheny, H., Tyree, T., Sabatini, D., and Klaine, J., 1988. Agricultural Runoff Modeling in a Small West Tennessee Watershed, Journal Water Pollution Control Federation. 60(2): 242-249.

Mostaghimi, S., Park, S. W., Cooke, R.A, and Wang S.Y., 1997. Assessment of Management Alternatives on a Small Agricultural Watershed. Water Research 31(8): 1867-1878.

Neitsch, S.L., Arnold, J.R., Kiniry, J.R., Williams, J.R., and King, W.K., 2002. Soil and Water Assessment Tool Theoretical Documentation Version 2000. Texas Water Resources Institute, College Station, Texas.

Northern Virginia Planning District Commission (NVPDC). 1994. Mission Statement for the Occoquan Basin Model Upgrade. Annandale, Virginia: Northern Virginia Planning District Commission.

Rahman, M., and Salbe, I., 1995. Modeling impacts of diffuse and point source nutrients on the water quality of South Creek catchment. Environment International. 21(5): 597-603.

Ravalico, J.K., Maier, H.R., Danday, G.C., Norton, J.P. , and Croke, B.F.W., 2005. A comparison of sensitivity analysis techniques for complex models for environment management. Proceedings of the International Congress on Modelling and Simulation, 2005/A. Zerger and R. M. Argent.

Saleh, A., and Du, B., 2004. Evaluation of SWAT and HSPF within BASINS Program for the Upper North Bosque river watershed in Central Texas. Transactions of the ASAE Vol. 47(4): 1039-1049.

Santhi, C., Arnold, J. G., Williams, J. R., Dugas, W. A., Srinivasan, R., and Hauck, L. M., 2001. Validation of the SWAT model on a large river basin with point and nonpoint sources. J. American Water Resources Assoc. 37(5): 1169−1188.

Shoemaker, C. A., and Benaman, J., 2003. A Methodology for Sensitivity Analysis in Complex Distributed Watershed Models. Philadelphia, PA, United States.

Suttles, J.B., Vellidis, G., Bosch, D., Lowrance, R., Sheridan, J.M., Usery, E.L., 2003. Watershed-scale simulation of sediment and nutrient loads in Georgia Coastal Plain streams using the Annualized AGNPS model. Trans. ASAE 2003, 46, 1325-1335.

Tang, Y., Reed, P., Wagener, T., and Van Werkhoven, K., 2007. Comparing sensitivity analysis methods to advance lumped watershed model identification and evaluation. Hydrology. Earth Syst. Sci., 11, 793-817.

Tsihrintzis, V.A., Fuentes, H.R., and Gadipudi, R.K., 1996. Modeling prevention alternatives for nonpoint source pollution at a Wellfield in Florida. American Resources Bulletin. 32(2): 317-331.

U.S. Environmental Protection Agency (USEPA), 2004. Users Manual for AQUATOX (Release 2): Modeling Environmental Fate and Ecological Effects in Aquatic Ecosystems Volume 1. EPA-823-B-04-001. Washington, D.C.: U.S. Environmental Protection Agency, Office of Water.

Vache, K. B., Eilers, J. M., and Santelmann, M. V., 2002. Water quality modeling of alternative agricultural scenarios in the U.S. corn belt. J. American Water Resources Assoc. 38(3): 773−787.

Walker, W. W., 1986. Empirical Methods for Predicting Eutrophication in Impoundments; Report 3, Phase III: Applications Manual. Technical Report E-81-9. Vicksburg, Miss.: U.S. Army Engineers Waterways Experiment Station.

White, K. L., and Chaubey, I., 2005. Sensitivity Analysis, Calibration, and Validations for a Multisite and Multivariable SWAT Model. Journal of American Water Resources Association 41(5):1077-1089.

Wool, T. A., Ambrose, R. B., Martin, J. L., and Cormer, E. A., 2003. Water Quality Analysis Simulation Program (WASP) Version 6.0 Draft: User's Manual. In. Atlanta, Georgia: U.S. Environmental Protection Agency.

Wu, J., 2004. Water-quality-based BMP design approach and uncertainty analysis for integrated watershed management. PhD. Dissertation, University of Virginia.

Xu, Z., 2005. A complex, linked watershed-reservoir hydrology and water quality model application for the Occoquan Watershed, Virginia. PhD. Dissertation, Virginia Tech

Xu, Z., Godrej, A.N., and Grizzard, T.J., 2007. The hydrological calibration and validation of a complexly-linked watershed-reservoir model for the Occoquan Watershed, Virginia. Journal of Hydrology, 345, 3–4: 167-183.

Young, R.A., Onstad, C.A., Bosch, D.D., and Anderson, W.P., 1994. Agricultural Non-Point Source Pollution Model, Version 4.03 AGNPS User's Guide. U.S. Department of Agriculture, Washington, D.C.

Yuan, Y., Mehaffey, M. H., Lopez, R. D., Bingner, R. L., Bruins, R. J., Erickson, C. L., and Jackson, M., 2011. AnnAGNPS Model Application for Nitrogen Loading Assessment for the Future Midwest Landscape Study. JOURNAL OF WATER SRT - AQUA. Blackwell Publishing, Malden, MA, 3(1):196-216.

Zheng Y., and Keller, A. A., 2006. Understanding parameter sensitivity and its management implications in watershed-scale water quality modeling. Water Resource. Res., 42, W05402.

Chapter 3. Sensitivity Analysis, Calibration and Validation of a Watershed Model Application using HSPF with the Nutrient Algorithm PQUAL in Upper Broad Run Watershed, Virginia

Yingmei Liu[1], Adil N. Godrej[2], and Thomas J. Grizzard[3]
[1]PhD graduate, Civil and Environmental Engineering, Virginia Tech, Manassas, VA
[2]Research Associate Professor, Civil and Environmental Engineering, Virginia Tech, Manassas, VA
[3]Professor, Civil and Environmental Engineering, Virginia Tech, Manassas, VA

To be submitted to *Journal* of the *American Water Resources Association* (JAWRA)

3.1 Abstract

A watershed model application using HSPF with the nutrient algorithm PQUAL was developed for Upper Broad Run, a 126.21 km^2 rural watershed in Fauquier County in Virginia. The model was calibrated for a four-year period (2002-2005) and validated for a two-year period (2006-2007). Based on annual, seasonal and monthly loading comparisons, the calibration and validation varied between very good and reasonable for flow, sediment and nutrients: OP (orthophosphate phosphorus), NH_4-N (ammonium nitrogen) and Ox-N (oxidized nitrogen).

“One-variable-at-a-time” sensitivity analysis, using the normalized sensitivity index (*S*), was performed on the calibrated model to examine the sensitivity of model outputs (flow, sediment and nutrient loadings) with respect to model inputs and parameters. Results were presented for both average yearly and average seasonal (spring, summer, fall, winter) values of the model outputs. Seven meteorological inputs and 47 parameters related to streamflow generation, sediment and nutrient transport, and interactions on lands and within streams were included in the sensitivity analysis.

Generally, all model outputs were quite sensitive to meteorological inputs, especially precipitation, indicating the importance of accurately representing climate conditions for the

watershed. The sensitivity analysis results confirmed that accurate hydrologic simulation is of first important because of its significant impact on sediment and nutrient loadings. In addition, the OP and NH_4-N loadings were sensitive to PQUAL parameters describing pollutant buildup and washoff at land surface. On the other hand, a significant PQUAL parameter for the Ox-N loading was groundwater nitrate concentration. Most of the sensitive inputs and parameters became a little more significant in summer, probably associated with intense storm events and higher ET (potential evapotranspiration). It was also found that most of the sensitive parameters were associated with flow, sediment and nutrient generation processes on lands. Parameters for in-stream processes only had significant impacts on sediment loading.

3.2 Introduction

In the U.S.A, excessive nutrients from agricultural activities and urban development have been identified as a leading cause of waterbody impairment (USEPA, 2002). Large amounts of nitrogen and phosphorus can cause eutrophication, with accelerated growth of algae, increased turbidity and reduced dissolved oxygen in the water. It thus impairs recreation, aesthetics, and other beneficial uses of the waterbody. For each impaired waterbody, nutrient TMDL (total maximum daily load) development is required under the Clean Water Act to improve water quality by reducing point and nonpoint source loadings.

As a comprehensive and continuous watershed model simulating hydrology and water quality processes on lands and within streams, the Hydrological Simulation Program-FORTRAN (HSPF) has been widely used for watershed nutrient simulation (for example, Rahman and Salbe, 1995; Bergman et al., 2002; Liu et al.,2008). HSPF is also a very useful tool for estimating nutrient sources in support of nutrient TMDL development (Filoso et al., 2004; Shoemaker et al, 2005). One of the largest applications of HSPF is in the 64,000 square mile Chesapeake Bay watershed, which is used to determine total watershed contributions of flow, sediment and nutrients (Donigian et al., 1994) and evaluate water quality effects of nutrient and sediment reduction plans (Cerco et al., 2002).

HSPF simulates water, sediment and nutrients on pervious and impervious lands and within streams. Nutrient fate and transport from the previous lands can be simulated using two algorithms: PQUAL and AGCHEM. Of the two algorithms, PQUAL is easier to apply and generally used in watershed nutrient simulation (for example, Bergman et al., 2002; El-Kaddah and Carey, 2004; Xu, 2005). PQUAL assumes simple relationships of nutrient loads with water and sediment yield. With PQUAL, the nutrient loads from the previous lands are the summation of loads from land surface, interflow and groundwater. The nutrient simulation from the impervious lands is similar to PQUAL, but without subsurface processes.

Calibrating HSPF applications can be quite challenging, with over 100 parameters involved, particularly for some parameters without a straightforward connection to physical processes. In this context, it is very helpful to perform a sensitivity analysis (SA) to efficiently identify critical parameters, which require more attention in the parameter estimation. Besides improving model calibration, knowing how sensitive model outputs are with respect to input parameters might help with model selection, data collection planning, and model uncertainty analysis (Fontaine and Jacomino, 1997).

Over-parameterization and the complex nature of watershed models present challenges for efficient sensitivity analysis. Among the SA techniques (for example, nominal range sensitivity method, Monte Carlo method and generalized sensitivity analysis) for watershed models, "one-variable-at-a-time" sensitivity analysis (also called nominal range sensitivity method) is the most used one (Zheng and Keller, 2006).

A few studies have conducted the "one-variable-at-a-time" sensitivity analysis on HSPF, mostly for hydrology and sediment transport. Fontaine and Jacomino (1997) conducted SA to identify sensitive parameters of HSPF for the output variables including streamflow, flux of sediment and Cs^{137}on a 6.2 mi^2 catchment in eastern Tennessee. Parameters associated with streamflow generation, sediment transport and particle reactive contaminants on pervious lands and within streams were included in the sensitivity analysis. Donigian and Love (2007) performed SA on an HSPF application in the Housatonic River watershed to identify sensitive parameters for streamflow, TSS (total suspended solid) loading and water temperature. Besides model parameters, meteorological inputs (i.e., precipitation, air temperature and solar radiation) were also included in the sensitivity analysis. It was found that all the model outputs were most sensitive to the inputs of precipitation and/or air temperature, indicating the importance of accurate climate representations.

One preliminary sensitivity analysis was performed on HSPF parameters with respect to nutrient loadings in the Swift Creek Reservoir watershed, VA (Wu, 2004). The AGCHEM algorithm was used for nutrient simulation in the watershed. Some of the AGCHEM parameters describing nitrogen and phosphorus cycling in the soil were included in the sensitivity analysis. Despite the wide uses of PQUAL in HSPF applications for nutrient simulation, sensitivity analysis of nutrient fate and transport with such applications is not reported in literature. More information is clearly needed on this subject to provide a better guidance to model applications.

The principal objective of this paper was to evaluate sensitivity of HSPF with PQUAL for watershed nutrient simulation. The sensitivity analysis included meteorological inputs and parameters related to streamflow generation, sediment and nutrient transport and interactions. The study was conducted for the Upper Broad Run watershed, which is a rural and urbanizing watershed located in the larger Occoquan watershed in Northern Virginia. Integral to the objective was to develop, calibrate and validate the HSPF application in the study area. By identifying significant processes, inputs and parameters, the sensitivity analysis would provide useful information for model calibration, input data collection and preliminary uncertainty analysis. It is hoped that findings from this study will help with better application of HSPF with PQUAL for watershed nutrient simulation and nutrient TMDL development studies.

3.3 Materials and Methods

3.3.1 Study Area

The Upper Broad Run watershed is a 126.21 km^2 basin that lies in Fauquier County and drains to Lake Manassas, Virginia. The basin is located in the upper part of the larger Occoquan watershed in the Northern Virginia suburbs of Washington, DC (Figure 3-1). The stream station ST70 at the outlet of the basin, like other stream stations in the Occoquan watershed, has been monitored by the Occoquan Watershed Monitoring Laboratory (OWML) for both flow and water quality. Flow is measured continuously by automated equipment and recorded once per hour during baseflow conditions, and every 15 minutes during storm events. Water quality samples are both flow-weighted composite (storm) and grab samples (baseflow). Baseflow grab samples are taken on a biweekly basis during the winter season and on a weekly basis during other seasons. An effort is made to collect composite flow-weighted storm water quality samples automatically for all storms.

The climate in the study area is humid-subtropical with four distinctive seasons. The average annual air temperature and precipitation are about 13.2 ℃ and 101.6 cm, respectively. Meteorological data are collected at several sites in the Upper Broad Run watershed. Air temperature, cloud cover, dew point temperature, potential evapotranspiration (ET), solar radiation, and wind speed data are obtained from the Washington Dulles International Airport weather station (DULL in Figure 3-1). Precipitation data are obtained from AIRL (Airlie), RITC (C. Hunter Ritchie Elem. School), and CSNY (Camp Snyder wetlands), as shown in Figure 3-1.

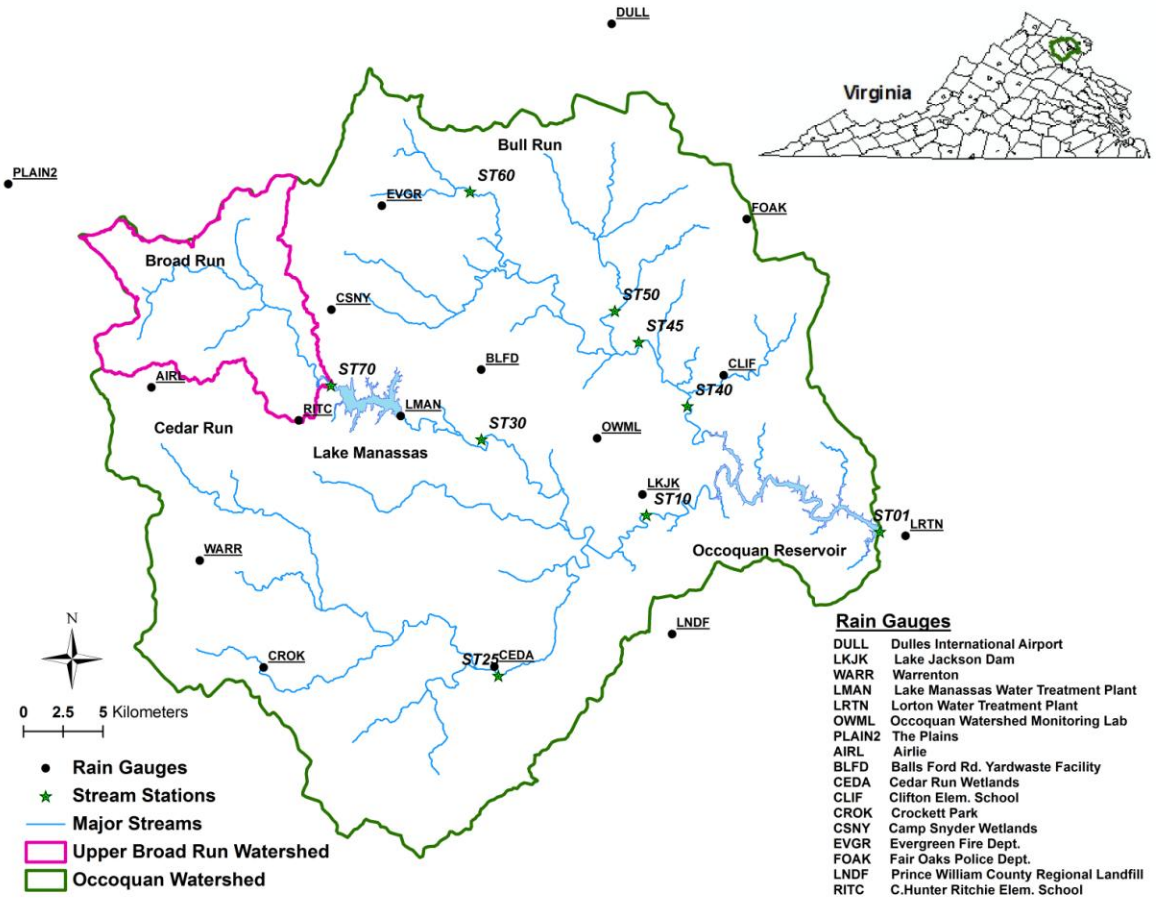


Figure 3-1: Location of Upper Broad Run Watershed, Showing Major Streams, Stream Stations and Rain Gauges in the Occoquan Watershed

The Upper Broad Run watershed is located in the Piedmont Region physiographic province, underlain by metamorphic rocks of diverse origins that can be traced back to the Paleozoic period (VDMR, 2001). Much of the study area falls into the Foothills subprovince, which has moderate slopes and relatively high elevation from 400 ft (121.92 m) to 1000 ft (304.8 m). The soils are generally loam and moderately well-drained. Based on the information from the State Soil Geographic (STATSGO) database, about 67% of the soils are categorized as B for the SCS (Soil Conservation Society) hydrological soil group, which features a moderate infiltration rate when thoroughly wetted.

The study area is a rural watershed that is undergoing continuous urbanization. Land use data are obtained from the Northern Virginia Regional Commission (NVRC), which determines land use every five to six years by reducing aerial photography. Based on the 2006 land use distribution, forest has the largest percentage (63.3%), followed by pasture (20.9%), cropland (9.9%), and urban (5.9%).

3.3.2 Model Development

As one of the core programs of the U.S. Environmental Protection Agency's (EPA) Better Assessment Science Integrating Point and Nonpoint Sources (BASINS) package, HSPF is a comprehensive, continuous, conceptual lumped model designed to simulate hydrology and water quality processes in a watershed (Bicknell et al., 2005). HSPF consists of three application modules—PERLND, IMPLND, and RCHRES—which simulate runoff and water quality constituents from pervious and impervious lands, and free flow reaches/well-mixed impoundments, respectively. Bicknell et al. (2005) and Donigian et al. (1995) provide detailed descriptions of these modules. The algorithms used for hydrology, sediment and nutrient simulation in this study are briefly described below.

Hydrology simulation

HSPF simulates a complete land-side water budget on pervious and impervious lands. Water budget on pervious lands accounts for precipitation, snowmelt, evapotranspiration, soil moisture storage, deep percolation, and outflow based on infiltration process and storage-capacity factors represented by empirical equations. Outflows from pervious lands are in three pathways: surface runoff, interflow, and groundwater (baseflow). Impervious lands, where no infiltration occurs, principally generate surface runoff. Water from surface runoff, interflow, or groundwater continues to be routed to streams by use of storage-volume relationships defined in FTABLEs (hydraulic function tables containing depth, surface area, volume, and flow information for reaches).

Sediment simulation

Overland sediment erosion and transport on pervious and impervious lands are simulated using exponential relationships for soil detachment and washoff. Within streams, sediment transport, deposition and scour are simulated for three classes: sand, silt, and clay. Non-cohesive (sand) sediment transport is simulated based on a sand-carrying capacity of the reach as a power function of the average flow velocity. Cohesive (silt, clay) sediment transport is simulated based on a bed shear stress as a function of the slope and hydraulic radius of the reach.

Nutrient simulation

HSPF provides two algorithms for nutrient simulation on pervious lands: a simpler empirical method PQUAL, or a more detailed physical method AGCHEM. In this model application, PQUAL is used to simulate three nutrient species: orthophosphate phosphorus (OP), ammonium nitrogen (NH_4-N) and oxidized nitrogen (Ox-N). The nutrient loads from the previous lands are the summation of loads from the land surface, interflow and groundwater. The nutrient simulation on impervious lands is similar to PQUAL, but without subsurface processes. The nutrient fluxes from the pervious and impervious lands are then directed to streams for a further simulation of nutrient transformations.

PQUAL simulates nutrient fluxes from land surface, interflow and groundwater by assuming simple relationships of nutrient with water and sediment yield (Figure 3-2). POTFW (washoff potency factor) is used to relate the nutrient yield to sediment removal from land surface. The nutrient yield from land surface is also estimated based on a function of storage quantity and overland flow, called “buildup and washoff.” During dry periods, HSPF assumes a linear relationship for the nutrient buildup with a user-defined accumulation rate (ACQOP) within the maximum storage capacity (SQOLIM). During wet periods, HSPF assumes the nutrient flux to be related to overland flow by a user-defined washoff rate (WSQOP). The nutrient fluxes in interflow and active groundwater are estimated by multiplying flow and user-defined concentrations (IFLW-CON and GRND-CON).

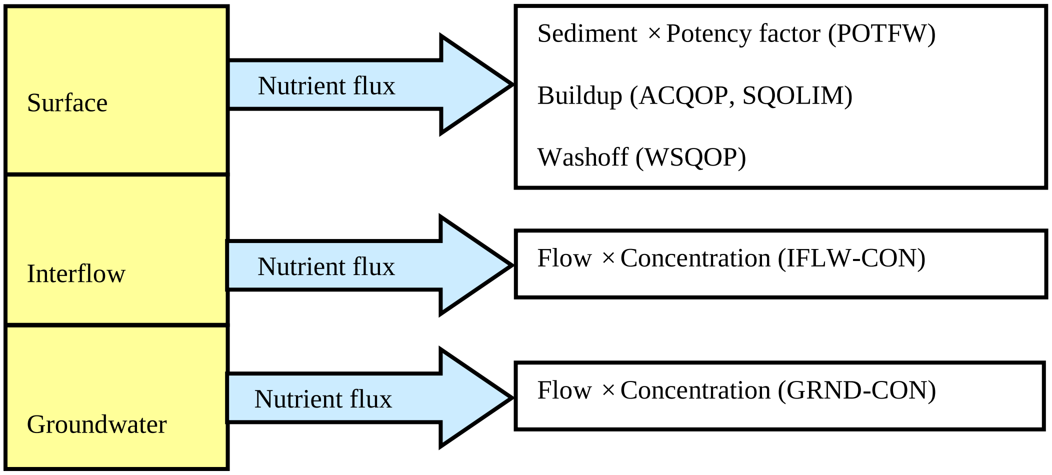


Figure 3-2: Nutrient Simulation by PQUAL

The HSPF application in the Upper Broad Run watershed was developed using 7 segments for the simulation period from 2002 to 2007 (Figure 3-3). Meteorological data were input on an hourly time step. The 2006 land use data were consolidated into nine land use categories for simulation: forest, pasture, high tillage cropland, low tillage cropland, townhouse/garden apartment, low density residential, medium density residential, industrial/commercial, and institutional. The categorization was based on land imperviousness and soil characteristics.

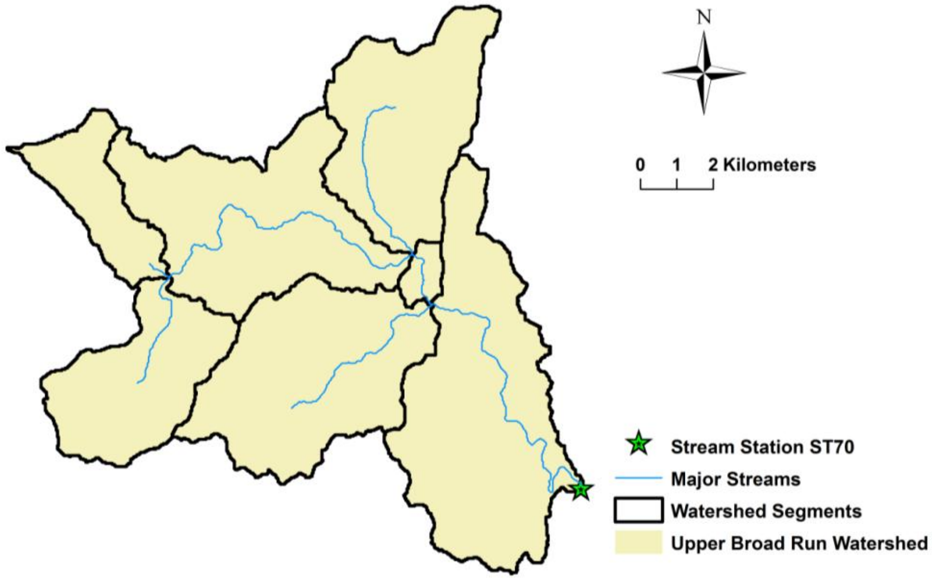


Figure 3-3: Segmentation of the Upper Broad Run Watershed

3.3.3 Model Calibration and Validation

The model was calibrated for the period 2002 to 2005 and validated for the period 2006 to 2007 using observed data from stream station ST70. A stepwise procedure was applied during the calibration. Generally, hydrology was calibrated first, then sediment calibration, and lastly water quality calibration (Donigian, 2002). The calibration focused on comparing simulated and observed flow volume, TSS and nutrient (OP, NH_4-N, Ox-N) loadings. Unlike the continuously measured flow rates, the observed daily sediment and nutrient loadings were estimated by multiplying flow rates and pollutant concentrations using a spreadsheet developed by Johnston et al. (2000). In the spreadsheet, two empirical methods were developed to estimate baseflow and storm loadings for the days without water quality samples. A daily flow-data integration (DFDI) method was used to fill in missing baseflow concentrations by assuming a linear relationship on the baseflow sampling array. To estimate the event mean concentrations (EMCs) for missing storms, empirical regression relationships between storm flow volumes and EMCs were developed.

The references used for parameter selection and value ranges for the calibration included BASINS technical notes (USEPA, 2000; USEPA, 2006), HSPF Application Guide (Donigian et al., 1984) and similar HSPF applications in the HSPFParm Database (Donigian et al., 1999). During calibration, parameter values were adjusted within recommended ranges to obtain a satisfactory agreement between simulated and observed data. Information from local studies and preliminary sensitivity analyses also helped with the calibration process.

The agreement between simulated and observed data was evaluated by visual and statistical comparisons on annual, seasonal and monthly scales during calibration and validation periods. The statistical comparisons were presented with percentage difference (PD) and the standard coefficient of determination (R^2). The percentage difference (PD) between simulated and observed data was defined as

$$PD = \frac{100 \cdot (Y - X)}{X} \% \qquad (1)$$

Where X is the observed value, and Y is the simulated value.

3.3.4 Sensitivity Analysis

During the calibration period, "one-variable-at-a-time" sensitivity analysis was performed to examine the sensitivity of model outputs with respect to meteorological inputs and parameters related to streamflow generation, sediment and nutrient transport and interactions. The primary outputs involved in SA were: flow, TSS loading, OP loading, Ox-N loading and NH_4-N loading. Each of the outputs was evaluated based on average annual values and average seasonal (spring, summer, fall, winter) values, resulting in 25 measures of sensitivity.

A sensitivity index was used to calculate and compare the results. The normalized form of the sensitivity index (S) was calculated as

$$S = \frac{\Delta y / y}{\Delta x / x} = \frac{(y_2 - y_1)/y}{(x_2 - x_1)/x} \qquad (2)$$

Where x is the base value of parameter, y is the base value of output, and x_2 and x_1 indicate a ±10% change of the parameter values, respectively. Correspondingly, y_2 and y_1 indicate the output responses to x_2 and x_1. Using a 10% variation is somewhat arbitrary but adequate for a standard sensitivity analysis (Fontaine and Jacomino, 1997).

S can be positive, zero or negative indicating positive correlation, no correlation, and negative correlation. The greater the absolute value, the more sensitive a model output is to a particular parameter (White and Chaubey, 2005).

3.4 Results and Discussion

Compared to the long-term average annual precipitation of 101.6 cm from 1951 to 2007, the calibration years 2002, 2004 and 2005 were near-average, while 2003 was a wet year with an annual precipitation of 135.9 cm (Table 3-1). The validation period had a near-average year 2006 and a dry year 2007, indicted by an annual precipitation of 73.4 cm.

Table 3-1: Rainfall Summary (2002-2007)

Year	Rainfall (cm)				
	Spring (March – May)	Summer (June – August)	Fall (September – November)	Winter (December –February)	Total
2002	34.1	22.1	30.2	10.7	97.0
2003	35.7	35.9	38.5	25.8	135.9
2004	25.1	31.5	35.7	13.9	106.1
2005	30.2	27.8	28.5	14.4	100.9
2006	13.1	28.6	40.2	12.3	94.2
2007	18.0	24.0	17.6	13.8	73.4
Long-Term Average (1951-2007)	26.2	29.6	25.3	20.5	101.6

3.4.1 Model Calibration and Validation Results

The simulated flow volume, TSS and nutrient (OP, Ox-N, NH_4-N) loadings were compared with observed ones on annual, seasonal and monthly basis, as shown in Table 3-2, 3-3 and 3-4, respectively.

Flow calibration was considered to be very good overall. Over the four-year calibration period, the total flow was underestimated by 4.2%, and the PD values of the annual flows ranged from –12.9% to +14.3% (Table 3-2). Temporal variations in flow were captured well, with PD values of the seasonal average flows from –11.7% to +12.1% (Table 3-3) and the R^2 of the monthly flows of 0.787 (Table 3-4) during the calibration period.

As the most difficult constituent to calibrate in HSPF (USEPA, 2006), sediment was predicted reasonably well. As shown in Table 3-2, the PD values of the annual TSS loadings in 2002 and 2003 were +9.5% and +6.3%, respectively. The relatively large PD value in 2005 (–53.7%, Table 3-2) was mainly due to under-prediction of TSS loadings for two closely-spaced storms in March 2005, which might also help to explain the relatively large error in predicting spring average TSS loading (–41.8%, Table 3-3) during the calibration period. The relatively low R^2 for monthly TSS loading was not unexpected as low correlation coefficients were often reported in other sediment modeling studies (for example, Engelmann et al., 2002; Saleh and Du, 2004).

The calibration of nutrient (OP, Ox-N, NH_4-N) loadings was considered to be very good based on annual comparisons. Over the four-year calibration period, the absolute PD values of the average annual nutrient loadings were 5.9% or less, and the PD values of the annual nutrient loadings for most years were within ±15% (Table 3-2). The temporal variations of OP and Ox-N loadings were captured well, indicated by low PD values based on seasonal comparisons (from –28.1% to +26.6%, Table 3-3) and high R^2 values based on monthly comparisons (0.604 for OP and 0.741 for Ox-N, Table 3-4). Comparatively, the seasonal and monthly comparisons of NH_4-N loading showed relatively weaker correlation.

A closer investigation was performed for simulated water balance during the calibration period, as shown in Table 3-5. The average annual water input from 2002 to 2005 was around 114.2 cm. Approximately 55.9% of the water input turned into evapotranspiration back to the hydrological cycle, and 31.7% became baseflow, which generally dominated the outflow from the watershed. Table 3-6 shows simulated nutrient flux from different pathways: surface, interflow and active groundwater (baseflow). 71.1% of OP and 67.6% of NH_4-N were transported overland, and 79.7% of Ox-N was transported in active groundwater (baseflow). In contrast to OP and NH_4-N, Ox-N is very mobile and easily leaches into water (Hantzsche and Finnemore, 1991).

Table 3-2: Annual Comparison by Variable and Year during Calibration and Validation Periods for the HSPF/PQUAL Application

	Calibration					Validation		
	2002	2003	2004	2005	Total (2002-2005)	2006	2007	Total (2006-2007)
Flow (10^6 m^3)	+14.3%	–8.4%	+5.4%	–12.9%	–4.2%	–3.6%	+12.4%	+2.2%
	(25.59/29.25)	(104.97/96.16)	(49.02/51.69)	(58.94/51.35)	(238.52/228.45)	(42.94/41.40)	(24.38/27.40)	(67.32/68.8)
TSS (10^9 g)	+9.5%	+6.3%	–30.0%	–53.7%	–18.8%	–50.0%	–20.7%	–43.3%
	(0.91/0.99)	(5.56/5.91)	(3.25/2.28)	(3.67/1.70)	(13.39/10.88)	(2.38/1.19)	(0.70/0.55)	(3.08/1.74)
OP (10^6 g)	+3.8%	–4.7%	+14.9%	–28.7%	–5.9%	–65.2%	–56.2%	–61.7%
	(0.31/0.33)	(1.78/1.70)	(0.69/0.79)	(0.85/0.60)	(3.63/3.42)	(0.94/0.33)	(0.60/0.27)	(1.54/0.60)
Ox-N (10^6 g)	+12.2%	+0.9%	+10.5%	+0.6%	+4.1%	+17.1%	+40.3%	+25.4%
	(18.23/20.46)	(70.27/70.88)	(34.05/37.61)	(37.14/37.35)	(159.69/166.3)	(25.24/29.57)	(13.99/19.62)	(39.23/49.19)
NH_4-N (10^6 g)	–38.4%	+6.1%	+4.8%	–11.4%	–3.1%	–40.6%	+15.2%	–24.9%
	(1.34/0.82)	(5.38/5.71)	(2.29/2.40)	(2.43/2.15)	(11.44/11.08)	(1.58/0.94)	(0.62/0.71)	(2.20/1.65)

Note: Values in ( ) below PD values are the observed and simulated flows or loads

Table 3-3: Seasonal Average Comparison by Variable during Calibration and Validation Periods for the HSPF/PQUAL Application

		Spring (March – May)	Summer (June – August)	Fall (September – November)	Winter (December –February)
Flow (10^6 m^3)	Calibration (2002-2005)	–11.7% (21.20/18.73)	–1.7% (10.10/9.93)	+12.1% (11.96/13.40)	–8.0% (16.37/15.05)
	Validation (2006-2007)	–6.4% (9.72/9.10)	+68.8% (3.20/5.41)	+12.3% (8.34/9.37)	–15.1% (12.39/10.53)
TSS (10^9 g)	Calibration (2002-2005)	–41.8% (1.61/0.94)	–20.5% (0.66/0.53)	–1.0% (0.55/0.55)	+36.2% (0.52/0.71)
	Validation (2006-2007)	–39.6% (0.43/0.26)	–77.6% (0.48/0.11)	–50.1% (0.54/0.27)	+142.2% (0.10/0.24)
OP (10^6 g)	Calibration (2002-2005)	+0.1% (0.31/0.31)	–28.1% (0.19/0.14)	–16.7% (0.20/0.17)	+15.5% (0.21/0.25)
	Validation (2006-2007)	–66.7% (0.24/0.08)	–53.8% (0.06/0.03)	–72.2% (0.32/0.09)	–33.5% (0.15/0.10)
Ox-N (10^6 g)	Calibration (2002-2005)	+8.0% (12.83/13.86)	+12.7% (6.11/6.89)	+26.6% (7.56/9.58)	–16.1% (13.42/11.26)
	Validation (2006-2007)	+29.7% (5.21/6.76)	+97.1% (1.74/3.43)	+63.3% (4.03/6.59)	–9.4% (8.63/7.82)
NH_4-N (10^6 g)	Calibration (2002-2005)	–7.7% (1.21/1.12)	–58.5% (0.63/0.26)	+49.8% (0.32/0.47)	+30.5% (0.71/0.92)
	Validation (2006-2007)	–22.4% (0.33/0.26)	–86.5% (0.26/0.03)	–35.0% (0.31/0.20)	+68.3% (0.20/0.33)

Note: Values in ( ) below PD values are the observed and simulated flows or loads

Table 3-4: Monthly R^2 by Variable during Calibration and Validation Periods for the HSPF/PQUAL Application

	Flow	TSS	OP	Ox-N	NH_4-N
Calibration (2002-2005)	0.787	0.308	0.604	0.741	0.474
Validation (2006-2007)	0.711	0.258	0.352	0.657	0.275

Table 3-5: Simulated Water Balance

	Average (cm)	Percentage
Inputs	**114.2**	**100.0%**
Outflow	**46.1**	**40.4%**
Surface runoff	2.3	2.0%
Interflow	7.6	6.7%
Baseflow	36.2	31.7%
Evapotranspiration	**63.8**	**55.9%**
Deep groundwater loss	**4.3**	**3.7%**

Table 3-6: Simulated Nutrient Loss

	OP		Ox-N		NH_4-N	
	Average (kg/ha)	Percentage	Average (kg/ha)	Percentage	Average (kg/ha)	Percentage
Nutrient flux at surface	0.054	71.1%	0.101	3.0%	0.244	67.6%
Nutrient flux in interflow	0.013	17.4%	0.577	17.3%	0.021	5.8%
Nutrient flux in baseflow	0.009	11.5%	2.656	79.7%	0.096	26.5%
Total	0.077	100.0%	3.334	100.0%	0.361	100.0%

As was done for model calibration, flow, sediment and nutrient validation was also performed by comparing observed and simulated data on annual, seasonal and monthly scales as indicated by PD (Table 3-2 and Table 3-3) and R^2 (Table 3-4). The flow validation results generally showed a similar good relationship between observed and simulated data to the calibration results, thus indicating a good flow prediction in the watershed. The model performance for sediment and nutrient (OP, Ox-N, NH_4-N) validation was not as good. TSS and OP loadings were generally under-predicted during the validation period, based on annual comparison (Table 3-2) and seasonal comparison (Table 3-3). One exception was noticed for a large over-prediction of TSS loading during winter, with PD value of +142.2% (Table 3-3). However, the TSS loading during winter was generally small compared to other seasons (Table 3-3) and thus had limited impact on the annual balance.

3.4.2 Sensitivity Analysis Results

A normalized sensitivity index (*S*) was calculated using Equation (2) on 7 meteorological inputs and 47 parameters for flow, TSS loading, OP loading, Ox-N loading and NH_4-N loading. Table 3-7 lists the 54 inputs and parameters involved in the sensitivity analysis, organized into three categories: meteorological inputs, PERLND parameters, and REACH parameters. The determination of the inputs and parameters was based on literature and past HSPF experience. For each parameter, the calibrated value was used as the base value. The sensitivity analysis for each input/parameter involved two model runs: changing the input/parameter from the base value by +10% (except AGWRC, which was changed to its maximum value of 0.999) and by –10%.

Of the 7 meteorological inputs and 47 parameters that were analyzed, only a subset had noticeable impacts on model outputs. Table 3-8 shows the subset of inputs and parameters with *S* greater than 0.1 for average annual flow, TSS loading, OP loading, Ox-N loading and NH_4-N loading. Inputs and parameters with *S* values greater than 0.5 were considered to be significant. That is, a total change of 20% (±10%) in input/parameter produces a change of 10% or more in model output.

Table 3-7: Meteorological Inputs and HSPF/PQUAL Parameters Included in the Sensitivity Analysis

Parameter	Description
	Meteorological inputs
PREC	Precipitation
ATEM	Air temperature
DEWP	Dew point temperature
WIND	Wind speed
SOLR	Solar radiation
CLOU	Cloud cover
EVAP	Potential Evaporation
	PERLND parameters
AGWRC	Base groundwater recession rate
INFILT	Index to the infiltration capacity of the soil
INTFW	Interflow inflow parameter
IRC	Interflow recession parameter
LZSN	Lower zone nominal storage
UZSN	Upper zone nominal storage
LZETP	Lower zone ET parameter
DEEPFR	Fraction of groundwater inflow which will enter deep (inactive) groundwater
JRER	Exponent in the soil detachment equation
KRER	Coefficient in the soil detachment equation
JSER	Exponent in the detached sediment washoff equation
KSER	Coefficient in the detached sediment washoff equation
POTFW-OP (NH_4, NO_3)	Washoff potency factor of OP (NH_4, NO_3)
ACQOP-OP (NH_4, NO_3)	Accumulation rate of OP (NH_4, NO_3) on the surface
SQOLIM-OP (NH_4, NO_3)	Maximum storage of OP (NH_4, NO_3) on the surface
WSQOP-OP (NH_4, NO_3)	Rate of surface runoff that will remove 90% of stored OP (NH_4, NO_3) per hour
IFLW-CON-OP (NH_4, NO_3)	Interflow OP (NH_4, NO_3) concentration
GRND-CON-OP (NH_4, NO_3)	Groundwater OP (NH_4, NO_3) concentration
	REACH parameters
KSAND	Coefficient in the sandload power function formula
EXPSND	Exponent in the sandload power function formula
TAUCS (silt, clay)	Critical bed shear stress for (silt, clay) scour
M (silt, clay)	Erodibility coefficient of (silt, clay)
TAUCD (silt, clay)	Critical bed shear stress for (silt, clay) deposition
KTAM20	Nitrification rate of ammonium at 20 ℃
KNO320	Nitrate denitrification rate at 20 ℃
KBOD20	BOD decay rate at 20 ℃
ADNHPM (sand, silt, clay)	Adsorption coefficients for NH_4 adsorbed to (sand, silt, clay)
ADPOPM (sand, silt, clay)	Adsorption coefficients for OP adsorbed to (sand, silt, clay)

Table 3-8: Sensitivity Index (*S*) of Average Annual Output Variables to HSPF/PQUAL Inputs and Parameters

Parameter	Description	Calibrated value	Flow	TSS	OP	Ox-N	NH_4-N
	Meteorological inputs						
PREC	Precipitation	Not applicable	+1.9	+4.5	+4.0	+2.0	+3.7
ATEM	Air temperature	Not applicable	–0.7	–1.6	–1.9	–0.8	–1.8
EVAP	Potential Evaporation	Not applicable	–0.5	–1.3	–1.0	–0.5	–0.9
DEWP	Dew point temperature	Not applicable			–0.2		–0.4
SOLR	Solar radiation	Not applicable			–0.2		–0.2
	PERLND parameters						
AGWRC	Base groundwater recession rate	0.92	–2.6	–3.6	–0.5	–2.6	–0.9
LZETP	Lower zone ET parameter	0.46-0.6**	–0.4	–0.7	–0.6	–0.4	–0.5
LZSN	Lower zone nominal storage	5	–0.1	–0.2	–0.3	–0.1	–0.3
UZSN	Upper zone nominal storage	0.4-0.62**	-0.1	–0.3	–0.3	–0.1	–0.3
INFILT	Index to the infiltration capacity of the soil	0.13-0.18*		–0.6	–1.1		–1.0
INTFW	Interflow inflow parameter	3		–0.5	–0.8		–0.8
JSER	Exponent in the detached sediment washoff equation	2		–0.7	–0.1		
KSER	Coefficient in the detached sediment washoff equation	1.6-2.6*		+0.2			
SQOLIM-OP	Maximum storage of OP on the surface	0.06			+0.4		
WSQOP-OP	Rate of surface runoff that will remove 90% of stored OP per hour	0.7			–0.4		
IFLW-CON-OP	Interflow OP concentration	0.015-0.055**			+0.1		-0.1
GRND-CON-NO_3	Groundwater NO_3 concentration	0.65-1.5**				+0.8	
IFLW-CON-NO_3	Interflow NO_3 concentration	0.65-1.5**				+0.2	
SQOLIM-NH_4	Maximum storage of NH_4 on the surface	0.1					+0.6
WSQOP-NH_4	Rate of surface runoff that will remove 90% of stored NH_4 per hour	0.12					–0.4
GRND-CON-NH_4	Groundwater NH_4 concentration	0.02-0.08**					+0.2
	REACH parameters						
TAUCS (silt)	Critical bed shear stress for silt scour	1.3		–1.8			
M (silt)	Erodibility coefficient of the silt	0.01		+0.6			
TAUCS (clay)	Critical bed shear stress for clay scour	1.3		–0.5			
M (clay)	Erodibility coefficient of the clay	0.01		+0.2			
KTAM20	Nitrification rate of ammonia at 20 ℃	0.05			-0.1		–0.4

* Varying by land use

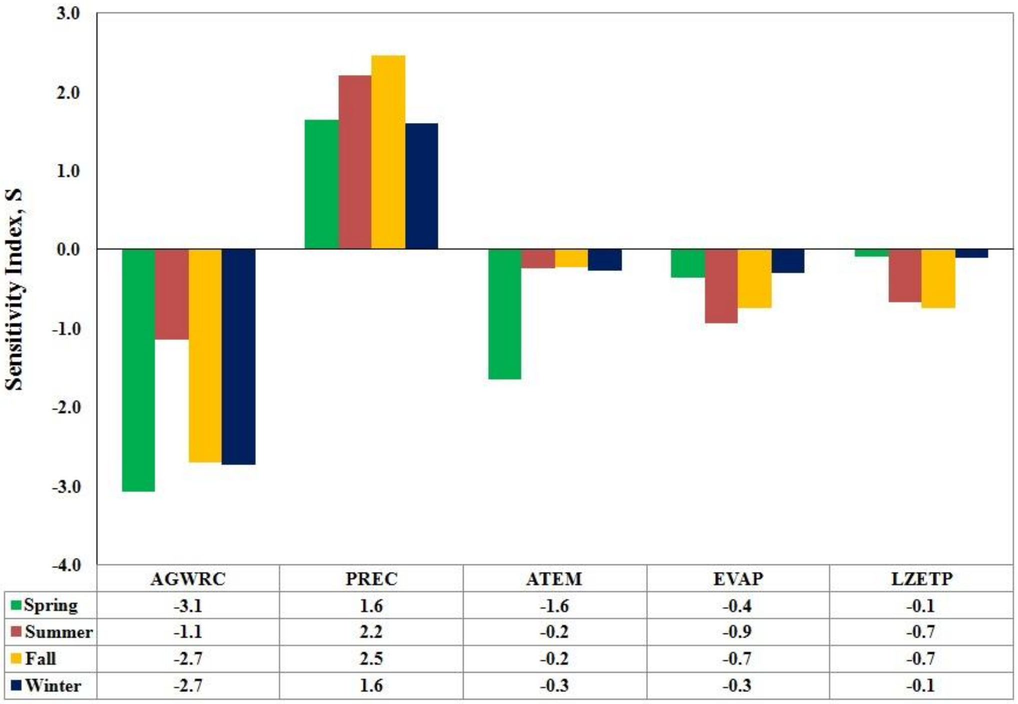
** Varying by month and land use

Figures 3-4, 3-5, 3-6, 3-7 and 3-8 show sensitivity index (*S*) for average seasonal (spring, summer, fall, winter) flow, TSS loading, OP loading, Ox-N loading and NH_4-N loading respectively. In each of the figures, only inputs and parameters with *S* greater than 0.5 for any of the seasonal average outputs are shown.

Flow sensitivity analysis

For the average yearly flow, the most sensitive parameter was AGWRC (base groundwater recession rate) with a sensitivity index of –2.6 (Table 3-8). AGWRC was negatively correlated with average yearly flow. By definition, AGWRC is the ratio of current groundwater discharge to that from 24 hours earlier. Increasing this parameter slows down the groundwater discharge. Possibly the streamflow was generally dominated by groundwater in this watershed (as shown in Table 3-5), so that AGWRC had a significant impact. As expected, precipitation (PREC) was the most sensitive meteorological input and positively correlated with the average yearly flow with a sensitivity index of +1.9 (Table 3-8). Less sensitive meteorological inputs included air temperature (ATEM) and potential evaporation (EVAP), which were negatively correlated with the average yearly flow (Table 3-8). As shown in Table 3-8, the average yearly flow was also negatively correlated with the lower zone ET (LZETP) and lower zone nominal storage (LZSN) parameters.

Seasonal sensitivity results were similar, except for a more significant impact of ATEM on average spring flow and less significant impact of AGWRC on average summer flow (Figure 3-4). In spring, snowmelt was an important component of flow generation, and air temperature involved in snow simulation became more significant. Summer flow was more sensitive to PREC than AGWRC when intense storms generated more surface runoff. In addition, EVAP and LZETP became relatively more important in summer and fall, with higher ET from vegetation (Figure 3-4).



	AGWRC	PREC	ATEM	EVAP	LZETP
🟩 Spring	-3.1	1.6	-1.6	-0.4	-0.1
🟥 Summer	-1.1	2.2	-0.2	-0.9	-0.7
🟨 Fall	-2.7	2.5	-0.2	-0.7	-0.7
🟦 Winter	-2.7	1.6	-0.3	-0.3	-0.1

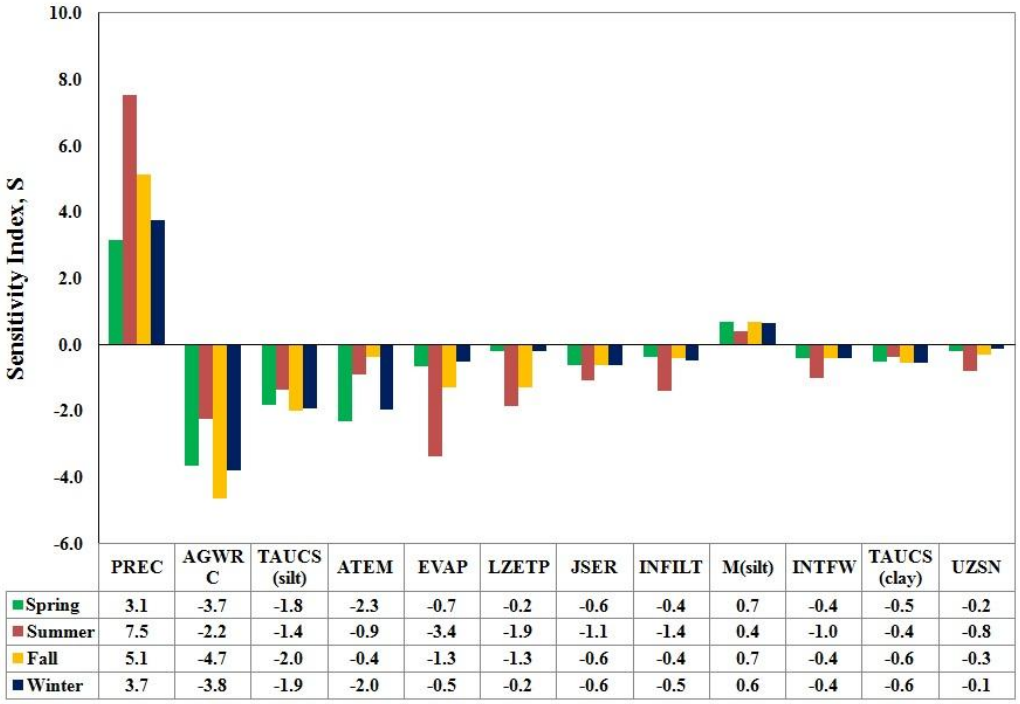
Figure 3-4: Sensitivity Index (*S*) of Average Seasonal Flow to HSPF/PQUAL Inputs and Parameters

Sediment sensitivity analysis

The average yearly TSS loading was very sensitive to meteorological inputs, especially precipitation, with a sensitivity index of +4.5 (Table 3-8). As shown in Table 3-8, the most sensitive parameter was AGWRC and less sensitive parameters included LZETP, INFILT (index to the infiltration capacity of the soil) and INTFW (interflow inflow). The results were understandable since sediment detachment and transport are closely associated with the flow process. Even though INFILT and INTFW were not sensitive parameters for average yearly flow, they had significant impacts (negative correlation) on sediment generation by controlling the amount of direct overland flow transporting the sediment. INFILT controls the overall moisture division between surface and subsurface (USEPA, 2000). Increasing INFILT produces less direct overland flow and more water in the lower zone and groundwater. INTFW determines the amount of water that enters the ground from surface detention storage and becomes interflow, as opposed to direct overland flow and upper zone storage (USEPA, 2000). Increasing INTFW causes an increase of interflow and decrease of direct overland flow.

Besides the flow generation processes, in-stream sediment processes had significant impacts on the average yearly sediment loading. The most sensitive REACH parameter was critical bed shear stress for silt scour (TAUCS) with a sensitivity index of –1.8 (Table 3-8). When it decreases, more sediment will be scoured from stream for transport. Overland sediment processes were less important than the in-stream sediment scour. Of the parameters describing the overland sediment processes, JSER (exponent in the detached sediment washoff equation) was relatively more important (Table 3-8).

Each of the average seasonal TSS loadings had similar sensitivity results. Compared to other seasons, most sensitive inputs and parameters became a little more significant in summer (Figure 3-5). For example, the average summer TSS loading was especially more sensitive to precipitation (S=+7.5, Figure 3-5) when the sediment generation was greatly affected by intense storm events. In summer, higher ET might significantly impact the flow process and thus played an important role in the sediment generation, indicated by the more significant impact of EVAP and LZETP during the season.



	PREC	AGWRC	TAUCS (silt)	ATEM	EVAP	LZETP	JSER	INFILT	M(silt)	INTFW	TAUCS (clay)	UZSN
🟩 Spring	3.1	-3.7	-1.8	-2.3	-0.7	-0.2	-0.6	-0.4	0.7	-0.4	-0.5	-0.2
🟥 Summer	7.5	-2.2	-1.4	-0.9	-3.4	-1.9	-1.1	-1.4	0.4	-1.0	-0.4	-0.8
🟨 Fall	5.1	-4.7	-2.0	-0.4	-1.3	-1.3	-0.6	-0.4	0.7	-0.4	-0.6	-0.3
🟦 Winter	3.7	-3.8	-1.9	-2.0	-0.5	-0.2	-0.6	-0.5	0.6	-0.4	-0.6	-0.1

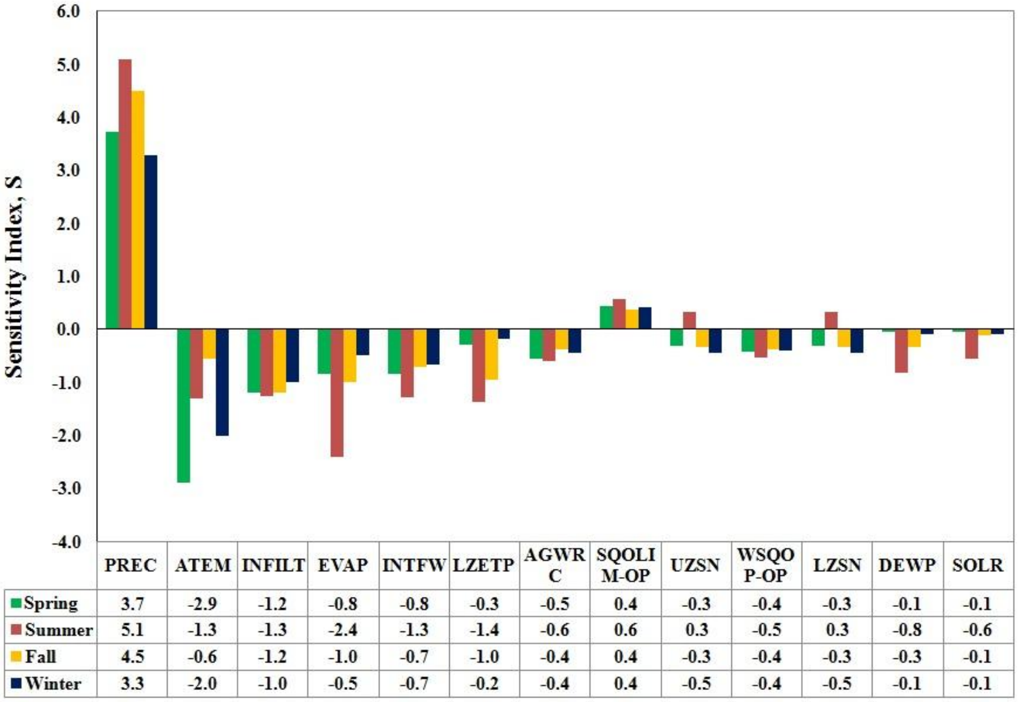
Figure 3-5: Sensitivity Index (*S*) of Average Seasonal TSS Loading to HSPF/PQUAL Inputs and Parameters

<u>Nutrient sensitivity analysis</u>

Similar to flow and sediment sensitivity results, the average annual nutrient (OP, Ox-N, NH_4-N) loading was also significantly impacted by meteorological inputs, especially precipitation (Table 3-8). Several important parameters describing the flow process had significant impacts on the average annual nutrient loadings. As shown in Table 3-8, the most sensitive parameter for the average annual Ox-N loading was AGWRC (S=–2.6), the key parameter to impact groundwater discharge. The most sensitive parameter for the average annual OP and NH_4-N loadings was INFILT (Table 3-8), which was closely related to overland flow generation. Another parameter (INTFW) controlling division between interflow and overland flow had significant impact on the average annual OP and NH_4-N loadings.

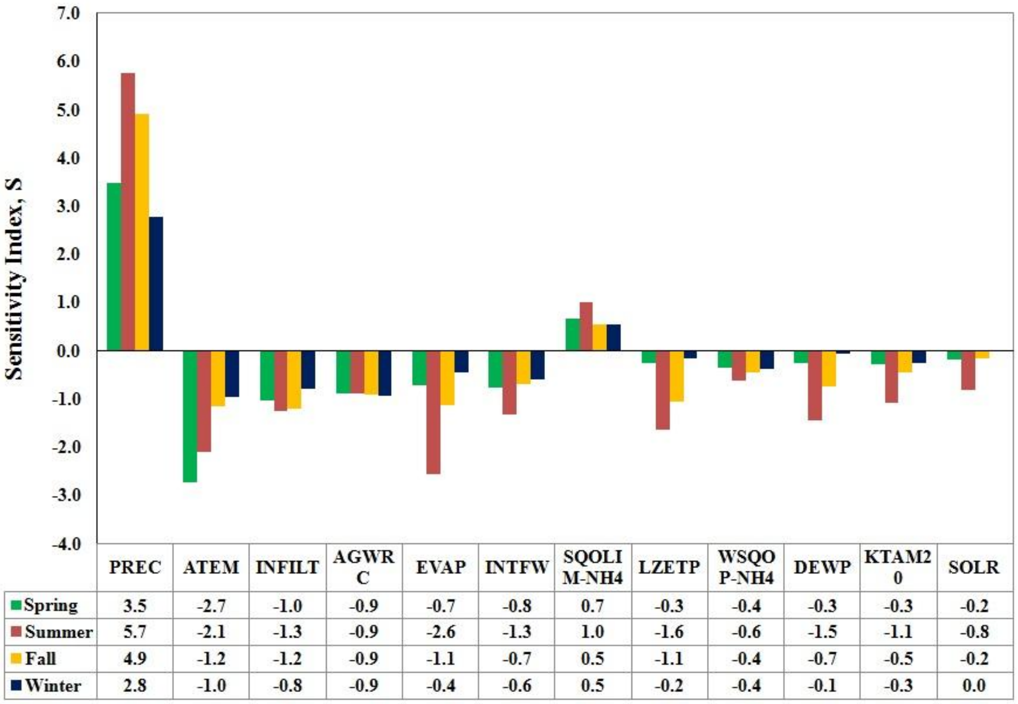
For the average annual OP loading, parameters describing overland buildup and washoff were relatively more important, including SQOLIM-OP (maximum storage of OP on the surface, *S*=+0.4, Table 3-8) and WSQOP-OP (rate of surface runoff that will remove 90% of stored OP per hour, *S*=–0.4, Table 3-8). SQOLIM-NH_4 and WSQOP-NH_4 were also found to be significant for the average NH_4-N loading, with sensitivity indices of +0.6 and –0.4, respectively. One possible reason was because OP and NH_4-N were mainly transported overland (as shown in Table 3-6), thus parameters describing pollutant buildup and washoff at land surface had significant impacts. This might also explain the significance of overland flow related parameters (INFILT and INTFW) on the average annual OP and NH_4-N loadings, as discussed earlier.

Figure 3-6 and 3-7 showed sensitivity results for average seasonal OP and NH_4-N loadings, similar to the annual sensitivity analysis. Additionally, most sensitive inputs and parameters (for example, PREC, EVAP and LZETP) became a little more significant in summer, probably associated with intense storm events and higher ET.



	PREC	ATEM	INFILT	EVAP	INTFW	LZETP	AGWRC	SQOLIM-OP	UZSN	WSQOP-OP	LZSN	DEWP	SOLR
🟩 Spring	3.7	-2.9	-1.2	-0.8	-0.8	-0.3	-0.5	0.4	-0.3	-0.4	-0.3	-0.1	-0.1
🟥 Summer	5.1	-1.3	-1.3	-2.4	-1.3	-1.4	-0.6	0.6	0.3	-0.5	0.3	-0.8	-0.6
🟨 Fall	4.5	-0.6	-1.2	-1.0	-0.7	-1.0	-0.4	0.4	-0.3	-0.4	-0.3	-0.3	-0.1
🟦 Winter	3.3	-2.0	-1.0	-0.5	-0.7	-0.2	-0.4	0.4	-0.5	-0.4	-0.5	-0.1	-0.1

Figure 3-6: Sensitivity Index (*S*) of Average Seasonal OP Loading to HSPF/PQUAL Inputs and Parameters

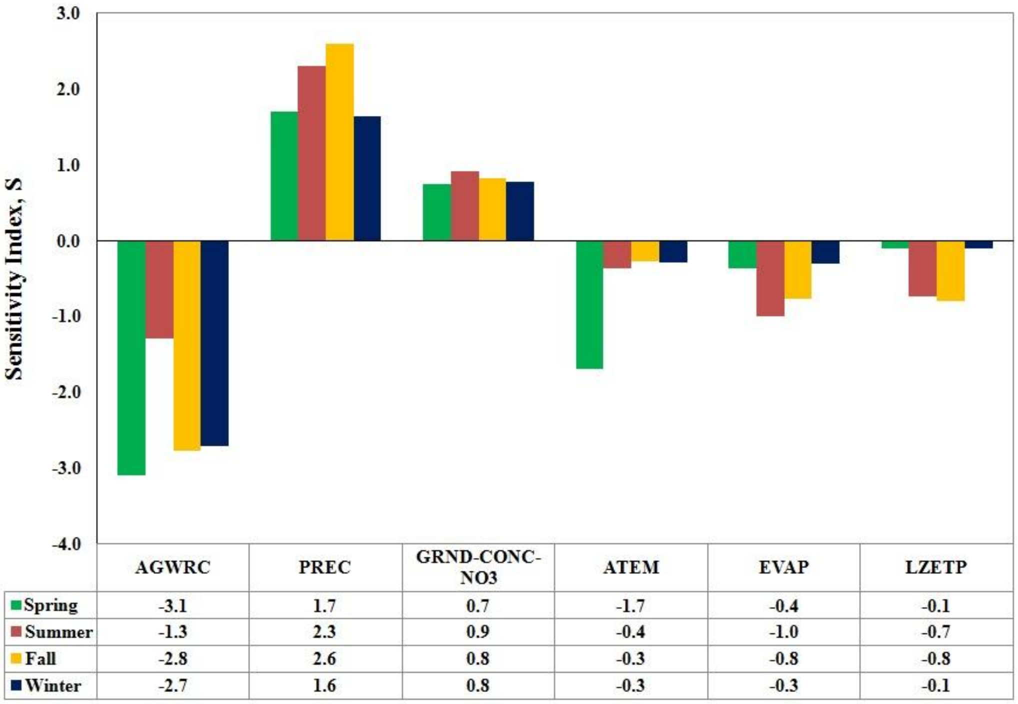


	PREC	ATEM	INFILT	AGWRC	EVAP	INTFW	SQOLIM-NH4	LZETP	WSQOP-NH4	DEWP	KTAM20	SOLR
🟩 Spring	3.5	-2.7	-1.0	-0.9	-0.7	-0.8	0.7	-0.3	-0.4	-0.3	-0.3	-0.2
🟥 Summer	5.7	-2.1	-1.3	-0.9	-2.6	-1.3	1.0	-1.6	-0.6	-1.5	-1.1	-0.8
🟨 Fall	4.9	-1.2	-1.2	-0.9	-1.1	-0.7	0.5	-1.1	-0.4	-0.7	-0.5	-0.2
🟦 Winter	2.8	-1.0	-0.8	-0.9	-0.4	-0.6	0.5	-0.2	-0.4	-0.1	-0.3	0.0

Figure 3-7: Sensitivity Index (*S*) of Average Seasonal NH_4-N Loading to HSPF/PQUAL Inputs and Parameters

Unlike for OP and NH_4-N, most Ox-N was transported in active groundwater, and groundwater nitrate concentration (GRND-CON-NO_3) was an important parameter for Ox-N simulation (*S*=+0.8, Table 3-8). This might also explain the significance of AGWRC (critical parameter controlling groundwater discharge) on the average annual Ox-N loading, as discussed earlier.

AGWRC had less significant impact on average summer Ox-N loading (Figure 3-8). Instead, PREC became more important than AGWRC in summer when intense storms generated more surface runoff. As shown in Figure 3-8, EVAP and LZETP also became relatively more important in summer, with higher ET from vegetation. In addition, ATEM involved in snowmelt simulation was found to have more significant impact on average spring Ox-N loading.



	AGWRC	PREC	GRND-CONC-NO3	ATEM	EVAP	LZETP
🟩 Spring	-3.1	1.7	0.7	-1.7	-0.4	-0.1
🟥 Summer	-1.3	2.3	0.9	-0.4	-1.0	-0.7
🟨 Fall	-2.8	2.6	0.8	-0.3	-0.8	-0.8
🟦 Winter	-2.7	1.6	0.8	-0.3	-0.3	-0.1

Figure 3-8: Sensitivity Index (*S*) of Average Seasonal Ox-N Loading to HSPF/PQUAL Inputs and Parameters

Given the shallow and quick-moving nature of streams, nutrient reaction parameters describing chemical and biological processes within streams generally won't have significant impacts on the nutrient loadings. When calibrating nutrient loadings, more attention might need to be given to the pollutant generation processes on land than the nutrient reactions in streams.

3.5 Conclusions

An HSPF model application (with the nutrient algorithm PQUAL) in the Upper Broad Run watershed was considered to provide a very good representation of flow and a reasonably good representation of sediment and nutrient loadings during the four-year calibration period (2002-2005) and two-year validation period (2006-2007). The validation results indicated that flow prediction was good, but appropriate judgment might be required for sediment and nutrient prediction.

Based on a closer investigation of the simulated water balance, the streamflow was generally dominated by active groundwater (baseflow) in the watershed. A closer investigation was also performed for the simulated nutrient flux from different pathways. It was found that OP and NH_4-N were mainly transported overland. On the other hand, most Ox-N was transported in active groundwater.

The sensitivities of model outputs (flow, sediment and nutrient loadings) with respect to 7 meteorological inputs and 47 parameters in the PERLND and REACH modules were evaluated with the normalized sensitivity index (S) during the calibration period. Only a subset of the inputs and parameters had noticeable impacts on the model outputs. Generally, all the model outputs were quite sensitive to meteorological inputs, especially precipitation, indicating the importance of accurately representing climate conditions for the watershed. The most sensitive parameter for streamflow was AGWRC, the key parameter controlling groundwater discharge in the PERLND module. The significant parameters for sediment loading included: 1) PERLND parameters associated with flow generation processes (i.e., AGWRC, LZETP, INFILT and INTFW); 2) REACH parameters associated with channel silt scour (i.e., TAUCS and M); 3) overland sediment transport parameter in the PERLND module (i.e., JSER). For OP and NH_4-N loadings, parameters describing overland flow generation (INFILT and INTFW), and pollutant buildup and washoff (SQOLIM and WSQOP) in the PERLND module were most significant On the other hand, the sensitive parameters for Ox-N loading included AGWRC and GRND-CON-NO_3 (groundwater nitrate concentration) in the PERLND module.

Almost none of the REACH parameters had significant impacts on flow and nutrient loadings. Therefore, more attention might need to be given to the land processes and parameters in the PERLND module while calibrating flow and nutrient loadings. It was also found that most sensitive inputs and parameters became a little more significant in summer, probably associated with intense storm events and higher ET. In addition, the significance of the parameters describing flow generation process on sediment and nutrient loadings illustrated the importance of accurate flow simulation for further model application.

Sensitivity of HSPF model outputs to parameters in any specific watershed depends on the combined impacts of climate and watershed conditions (Donigian and Love, 2007). Some of the sensitivity results could be applied to other studies with similar conditions. By identifying significant processes, inputs and parameters, this kind of sensitivity analysis would provide useful information for guiding HSPF usage.

3.6 References

Bergman, M.J., Green, W., and Donnangelo, L.J., 2002. Calibration of storm loads in the south Prong watershed, Florida, using BASINS/HSPF. Journal of the American water resources association. 38(5): 1423-1236.

Bicknell, B.R., Imhoff, J.C., Kittle, J.L., Jobes, T.H., and Donigian, A.S, 2005. Hydrological Simulation Program -Fortran (HSPF). User’s manual for release 12.2. U.S.EPA. National Exposure Research Laboratory, Athens, GA.

Cerco, C.F., Linker, L., Sweeney, J., Shenk, G. and Butt, A.J., 2002. Nutrient and Solid Controls in Virginia’s Chesapeake Bay Tributaries. Journal of Water Resources Planning and Management, 128(3): 179-189.

Donigian, A.S., Imhoff, J.C., Bicknell, B.R., and Kittle, J.L., 1984. Application Guide for Hydrological Simulation Program - Fortran (HSPF). U.S. EPA-600/3-84-065, Environmental Research Laboratory, Athens, GA.

Donigian, A. S., Bicknell, B. R., Patwardham, A. S., Linker, L. C., and Chang, C., 1994. Chesapeake Bay Program: watershed model application to calculate bay nutrient loadings. U.S. EPA-903-R-94-042, Chesapeake Bay Program Office. U.S.EPA. Annapolis, Maryland.

Donigian, A. S., Bicknell, B. R., and Imhoff, J. C., 1995. Hydrologic Simulation Program - FORTRAN. Computer Models of Watershed Hydrology, Water Resources Publications, V. P. Sirgh, ed., Highlands Ranch, CO, 395-442.

Donigian, A. S., Imhoff, J.C., and Kittle, J.L., 1999. HSPFParm, An Interactive Database of HSPF Model Parameters. Version 1.0. EPA-823-R-99-004. Prepared for U. S. EPA, Office of Science and Technology, Washington, D. C.

Donigian, A. S., 2002. Watershed Model Calibration and Validation: The HSPF Experience. National TMDL Science and Policy Specialty Conference 2002, Phoenix, Arizona, Water Environment Federation.

Donigian, A.S., and Love, J.T., 2007. The Housatonic River Watershed Model: Model Application and Sensitivity/Uncertainty Analysis. 7th International IWA Symposium on System Analysis and Integrated Assessment in Water Management, May 7-9, 2007. Washington, DC.

Engelmann, C. J. K., Ward, A. D., Christy, A. D., and Bair, E. S., 2002. Application of the BASINS database and NPSM model on a small Ohio watershed. J. American Water Resources Assoc.38(1): 289−300.

El-Kaddah, D.N., and Carey, A.E., 2004. Water quality modeling of the Cahaba River, Alabama. Environmental Geology. 45: 323-338.

Filoso, S., Vallino, J., Hopkinson, C., Rastetter, E., and Claessens, L. 2004. Modeling Nitrogen Transport in the Ipswich River Basin, Massachusetts, using a Hydrological Simulation Program Fortran (HSPF). Journal of the American Water Resources Association 40 (5): 1365–1384.

Fontaine, T. A., and Jacomino, V. M. F, 1997. Sensitivity analysis of simulated contaminated sediment transport. JAWRA 33: 313-326.

Hantzche, N. N., and Finnemore, E.J., 1991. Predicting ground-water nitrate-nitrogen impacts. Groundwater, 30 (4): 490-499.

Johnston, C.A., Grizzard, T.J., Godrej, A.N, and Post, H., 2000. Comparison of Two Tributary Pollutant Loading Rate Calculation Methods Using Continuous and Discrete Monitoring Data. Unpublished.

Liu, Z., Kingery, W.L., Huddleston, D. H., Hossain, F., Hashim N. B., and Kieffer J. M., 2008. Application and evaluation of two nutrient algorithms of Hydrological Simulation Program Fortran in Wolf River watershed. Journal of Environmental Science and Health, Part A 43(7):738-48.

Rahman, M. and Salbe, I. 1995. Modeling impacts of diffuse and point source nutrients on the water quality of South Creek catchment. Environment International. 21(5): 597-603.

Saleh, A., and Du, B., 2004. Evaluation of SWAT and HSPF within BASINS Program for the Upper North Bosque river watershed in Central Texas, Transactions of the ASAE Vol. 47(4): 1039-1049.

Shoemaker, L., Dai, T., Koenig, J., and Hantush, M., 2005. TMDL model evaluation and research needs. EPA/600/R-05/149.Cincinnati, Ohio: U.S. EPA, National Risk Management Research Laboratory.

United States Environmental Protection Agency (USEPA), 2000. BASINS Technical Note 6: Estimating Hydrology and Hydraulic Parameters for HSPF. EPA-823-R00-012, Washington, DC.

United States Environmental Protection Agency (USEPA), 2002. National Water Quality Inventory 2000 Report. EPA-841-R-02-001, Washington, DC.

United States Environmental Protection Agency (USEPA), 2006. BASINS Technical Note 8: Sediment Parameter and Calibration Guidance for HSPF. Office of Water, 4305, Washington, DC.

Virginia Division of Mineral Resource (VDMR), 2001. Geology of Virginia. Available at http://www.mme.state.va.us/DMR/DOCS/Geol/vageo.html. Accessed 17 August, 2007.

White, K. L. and Chaubey, I., 2005. Sensitivity Analysis, Calibration, and Validations for a Multisite and Multivariable SWAT Model. Journal of American Water Resources Association 41(5):1077-1089.

Wu, J., 2004. Water-quality-based BMP design approach and uncertainty analysis for integrated watershed management. PhD. Dissertation, University of Virginia.

Xu, Z., 2005. A complex, linked watershed-reservoir hydrology and water quality model application for the Occoquan Watershed, Virginia. PhD. Dissertation, Virginia Tech.

Zheng Y., and Keller, A. A., 2006. Understanding parameter sensitivity and its management implications in watershed-scale water quality modeling. Water Resource., Res., 42, W05402.

Chapter 4. Application and Sensitivity Analysis of a Watershed Model Application using HSPF with the Nutrient Algorithm AGCHEM in Upper Broad Run Watershed, Virginia

Yingmei Liu[1], Adil N. Godrej[2], Thomas J. Grizzard[3] and Theo Dillaha[4]
[1]*PhD graduate, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*
[2]*Research Associate Professor, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*
[3]*Professor, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*
[4]*Professor, Biological Systems Engineering, Virginia Tech, Blacksburg, VA*

To be submitted to *Journal* of the *American Water Resources Association* (JAWRA)

4.1 Abstract

A watershed model application using HSPF with the nutrient algorithm AGCHEM was developed, calibrated for a four-year period (2002-2005) and validated for a two-year period (2006-2007) in Upper Broad Run, a 126.21 km^2 rural watershed in Fauquier County in Virginia. Extensive effort was spent on estimating fertilizer and manure related nutrient inputs for the AGCHEM application. The nutrient simulation was considered reasonably well based on comparing simulated and observed OP (orthophosphate phosphorus) loading, NH_4-N (ammonium nitrogen) loading and Ox-N (oxidized nitrogen) loading on annual, seasonal and monthly scales.

"One-variable-at-a-time" sensitivity analysis was performed for the calibrated model to examine the sensitivity of nutrient (NH_4-N, Ox-N, OP) loadings with respect to model inputs and parameters, including: 7 meteorological inputs, 4 nutrient inputs (atmospheric, manure and fertilizer application rates, and fertilizer application time) and 103 parameters related to streamflow generation, sediment and nutrient transport and interactions on lands and within streams. The sensitivity analysis was performed based on both average yearly and average seasonal (spring, summer, fall, winter) values of the nutrient loadings.

Generally, the nutrient loadings were quite sensitive to meteorological inputs, especially precipitation, indicating the importance of accurately representing climate conditions for the watershed. Fertilizer application was found to be very important for the nutrient load generation. The nutrient loadings were positively correlated with the fertilizer application rate. Changing fertilizer application time showed significant impacts on seasonal nutrient loadings. Of the AGCHEM parameters describing nitrogen cycle in the soil, the NH_4-N loading was quite sensitive to the parameters describing ammonium adsorption and desorption in groundwater layer. On the other hand, the Ox-N loading was more sensitive to plant uptake of nitrogen. Phosphorus adsorption and desorption in upper layer was relatively more important for the OP load generation.

In addition, flow generation related parameters were found to have significant impact on the nutrient loadings. An accurate flow simulation is important for further model application. It was also found that most sensitive inputs and parameters became a little more significant in summer, probably associated with intense storm events and higher ET (potential evapotranspiration).

4.2 Introduction

In the U.S.A, excessive nutrient source from agricultural activities and urban development has been identified as one leading cause of waterbody impairment (USEPA, 2002). Large amounts of nutrients, primarily nitrogen and phosphorus, can cause waterbody eutrophication with harmful impacts on recreation, aesthetics, and other beneficial uses of the water. These impacts include algae blooms, high turbidity, low dissolved oxygen (DO) and fish kills. To address this issue, TMDLs (total maximum daily load) is required under the Clean Water Act for each impaired waterbody included in the State 303 (d) List.

Numerous watershed models have been developed and widely applied in simulating nutrient transport and fate in watersheds, such as Agricultural Non-Point-Source

Pollution Model (AGNPS) (Young, et al. 1994), Soil and Water Assessment Tool (SWAT) (Neitsch, et al. 2002) and Hydrological Simulation Program-FORTRAN (HSPF) (Bicknell et al., 2005). One of the important uses of the watershed models is to estimate nutrient sources in support of nutrient TMDL development (Borah et al. 2006). HSPF is one of the most extensively used models for watershed nutrient simulation (Shoemaker et al, 2005). HSPF simulates nutrient transport and fate on pervious and imperious lands and within streams. There are two algorithms for nutrient simulation on pervious lands: a simpler empirical method, PQUAL, and a more detailed physical method, AGCHEM. The AGCHEM algorithm applies a nutrient balance approach as the foundation for simulating complex nutrient processes in the soil explicitly, including the soil nutrient storage; nutrient input from atmospheric deposition, fertilization and manure application; and subsequent nutrient movement and transformation as well as plant uptake in the soil profile. Compared to PQUAL, AGCHEM has attractive features such as simulation of interactions between nutrient species and tracing of nutrient sources. Considering the capabilities, AGCHEM has been used for nutrient simulation in many HSPF applications (for example, Donigian et al., 1994; Im et al., 2003; Saleh and Du, 2004; Liu et al., 2008).

Extensive inputs and parameters are required during AGCHEM application to represent the complicated physical, chemical and biological processes in the soil profile. In some cases, estimating the inputs and parameters might involve many uncertainties and impact simulation significantly. For example, nutrient input estimates based on current or historical fertilization practices were found to generate quite different nutrient loadings in the Wolf River Watershed (Liu et al., 2005). Moreover, over-parameterization and the complex nature of the AGCHEM algorithm present challenges for model calibration. In this context, it is very helpful to perform a sensitivity analysis (SA) to efficiently identify critical parameters that require more attention in parameter estimation. Besides improving model calibration, knowing key processes, inputs and parameters might help with model selection, data collection planning, and model uncertainty analysis (Fontaine and Jacomino, 1997).

A few studies have conducted sensitivity analysis on HSPF, mostly for hydrology and sediment transport (for example, Fontaine and Jacomino, 1997; Donigian and Love, 2007). One preliminary sensitivity analysis was performed on HSPF parameters with respect to nutrient loadings in the Swift Creek Reservoir watershed (Wu, 2004). Non-point sources of nutrients in the watershed originated from fertilizer and manure applied on agricultural and residential areas. AGCHEM was used for nutrient simulation and some of the AGCHEM parameters describing nitrogen and phosphorus cycle in the soil were included in the sensitivity analysis. The study didn't include the fertilizer and manure inputs in the sensitivity analysis. To the best of our knowledge, a thorough sensitivity analysis of HSPF with AGCHEM for watershed nutrient simulation has not been reported in literature.

The principal objective of this paper was to evaluate sensitivity of HSPF with AGCHEM for watershed nutrient simulation. "One-variable-at-a-time" sensitivity analysis was performed to examine the sensitivity of nutrient loadings with respect to model inputs and parameters, including meteorological inputs, nutrient inputs and parameters related to streamflow generation, sediment and nutrient transport and interactions on lands and within streams. To conduct the sensitivity analysis, a watershed model application using HSPF with the nutrient algorithm AGCHEM was developed, calibrated for a four-year period (2002-2005) and validated for a two-year period (2006-2007) in the Upper Broad Run watershed, which is a rural and urbanizing watershed in Fauquier County in Northern Virginia. It is hoped that findings from this study will help with better application of HSPF with AGCHEM for watershed nutrient simulation and nutrient TMDL development studies.

4.3 Materials and Methods

4.3.1 Study Area

The Upper Broad Run watershed is located in the upper part of the larger Occoquan watershed in the Northern Virginia suburbs of Washington, DC (Figure 4-1). The Upper Broad Run flows into Lake Manassas and drains a 126.21 km^2 area in Fauquier County. The climate in the study area is humid-subtropical with four distinctive seasons. The average annual air temperature and precipitation are about 13.2 ℃ and 101.6 cm, respectively.

Most of the study area falls into the Foothills subprovince in the Piedmont Region physiographic province, characterized by moderate slopes and relatively high elevations from 400 ft (121.92 m) to 1000 ft (304.8 m). The soils are generally loam and moderately well-drained. Even though it is undergoing continuous urbanization, the study area is considered relatively undeveloped. Based on 2006 land use data from the Northern Virginia Regional Commission (NVRC), forest has the largest coverage (63.3%), followed by pasture (20.9%), cropland (9.9%), and urban (5.9%). The major grass is cool season turf grass including tall fescue grass and Kentucky blue grass. The main crops are hay, corn, wheat and soybean.

The stream station ST70 (as shown in Figure 4-1) at the outlet of the Upper Broad Run watershed is monitored by the Occoquan Watershed Monitoring Laboratory (OWML) for flow and water quality during baseflow conditions and storm events. Water quality samples during storm events are flow-weighted composites. At baseflow conditions, water quality grab samples are taken on a weekly basis, except for biweekly sampling during the winter season.

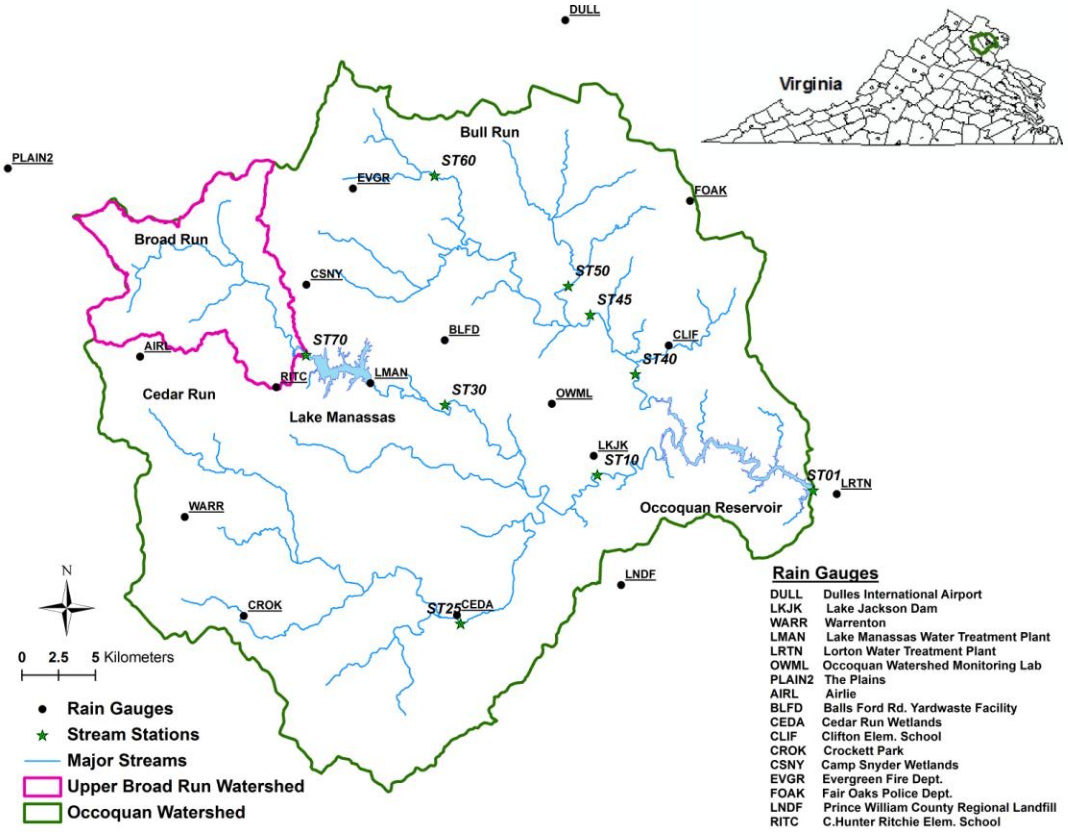


Figure 4-1: Location of Upper Broad Run Watershed, Showing Major Streams, Stream Stations and Rain Gauges in the Occoquan Watershed

4.3.2 Model Development

In the Upper Broad Run watershed, one HSPF application using the nutrient algorithm PQUAL was previously developed in the simulation period from 2002 to 2007 (Liu et al., 2011a). The watershed was simulated using 7 segments for the HSPF application (Figure 4-2).

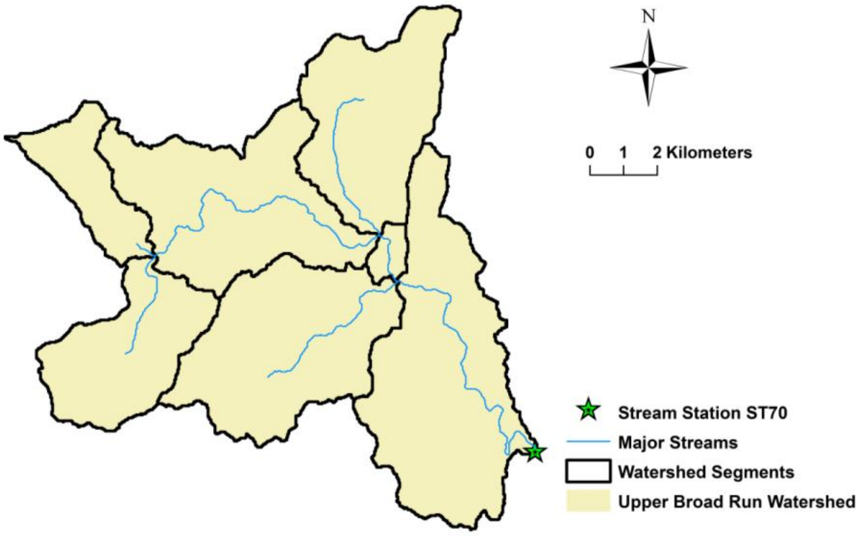


Figure 4-2: Segmentation of the Upper Broad Run Watershed

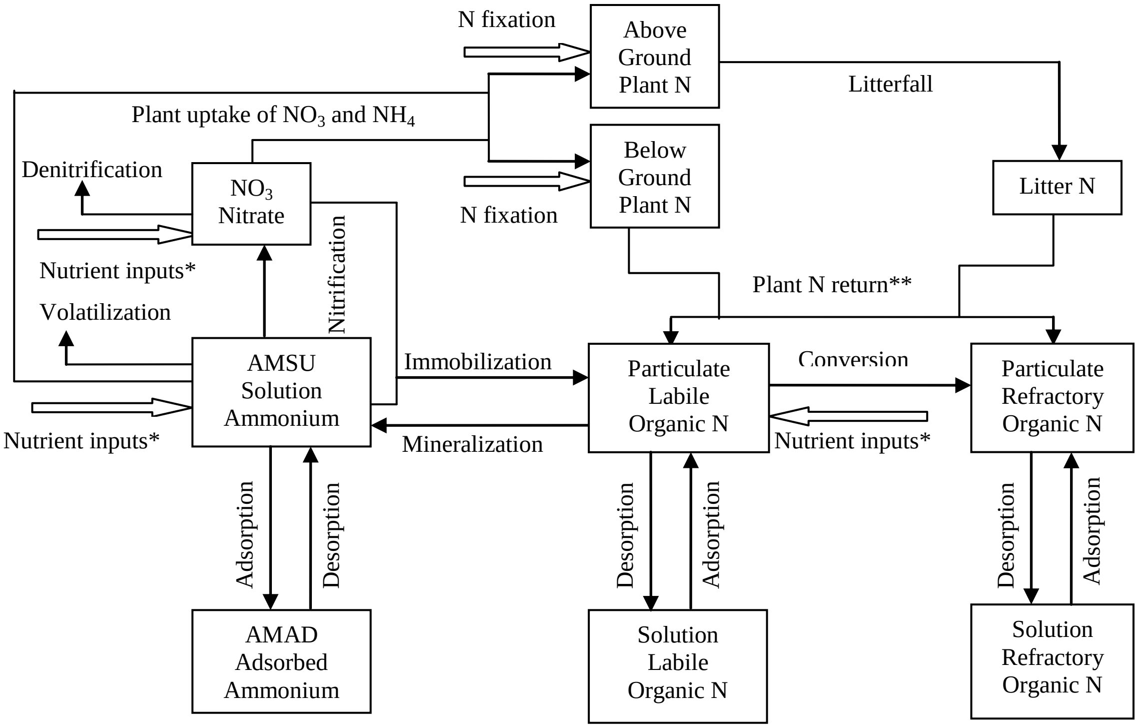
Meteorological data for the HSPF application included air temperature, cloud cover, dew point temperature, potential evapotranspiration (ET), solar radiation, wind speed, and precipitation. Except precipitation, other meteorological data were obtained from the Washington Dulles International Airport weather station (DULL in Figure 4-1). Precipitation data were obtained from AIRL (Airlie), RITC (C. Hunter Ritchie Elem. School), and CSNY (Camp Snyder wetlands), as shown in Figure 4-1. Meteorological data were input on an hourly time step.

The 2006 land use data from NVRC were consolidated into nine land use categories based on land imperviousness and soil characteristics: forest, pasture, high tillage cropland, low tillage cropland, townhouse, low density residential (LDR), medium density residential (MDR), industrial, and institutional.

In this research, the PQUAL application by Liu et al. (2011a) was replaced with the detailed process-based algorithm AGCHEM for watershed nutrient simulation. Three sections of AGCHEM including MSTLAY, NITR and PHOS were activated. Bicknell et al (2005) provide detailed description of these sections. Briefly, the MSTLAY section estimates the storage and fluxes of moisture in the soil profile, while the NITR and PHOS sections simulate nitrogen and phosphorus transport and soil reactions respectively, as shown in Figures 4-3 and 4-4. The soil profile is divided into four layers for moisture and nutrient storage, including surface, upper, lower and groundwater. The surface layer is shallow topsoil important for estimating surface runoff and sediment erosion, and the upper layer typically corresponds with the incorporation depth of fertilization (Kieffer, 2002). The lower layer where most of the plant transpiration occurs is typically determined based on the maximum depth of the crop root zone (Liu, 2006). The groundwater layer can be considered a mixing depth within the surface aquifer that controls the nutrient reactions and associated contributions to baseflow concentrations (Donigian, 1994). Soil layer depths shown in Table 4-1 were used for the AGCHEM application in the Upper Broad Run watershed.

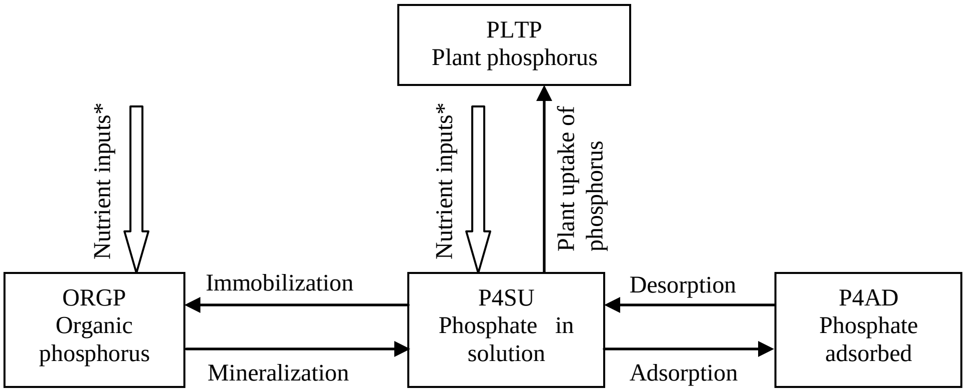
Table 4-1: Soil Layer Depths for the AGCHEM Application in the Upper Broad Run Watershed

Soil layer	Layer thickness (cm)	Bottom depth from soil surface (cm)
Surface	1.0	1.0
Upper	14.2	15.2
Lower	104.9	119.1
Groundwater	152.4	271.5



* Nutrient inputs from atmospheric deposition, fertilization and manure application
**Return of above ground plant N and litter N occurs to surface and upper layers only

Figure 4-3: Flow Diagram for Nitrogen Reactions by NITR (redrawn from Bicknell et al., 2005)



* Nutrient inputs from atmospheric deposition, fertilization and manure application

Figure 4-4: Flow Diagram for Phosphorus Reactions by PHOS (redrawn from Bicknell et al., 2005)

Crop representation for the AGCHEM application

Several factors (for example, planting and harvesting dates, fertilization and manure applications, plant uptakes of nutrients and erosion-related cover) involved in development of an AGCHEM application vary for different crops. For a better AGCHEM application, the high and low tillage croplands for the PQUAL application were split into hay, high tillage corn, low tillage corn, wheat, and soybean. The main difference between the high and low tillage corn was related to the erosion-related cover. The crop land areas were estimated using the high and low tillage crop distributions in Fauquier County (Figure 4-5) based on 2002 Census of Agriculture from USDA National Agricultural Statistics Service (NASS) (USDA, 2004).

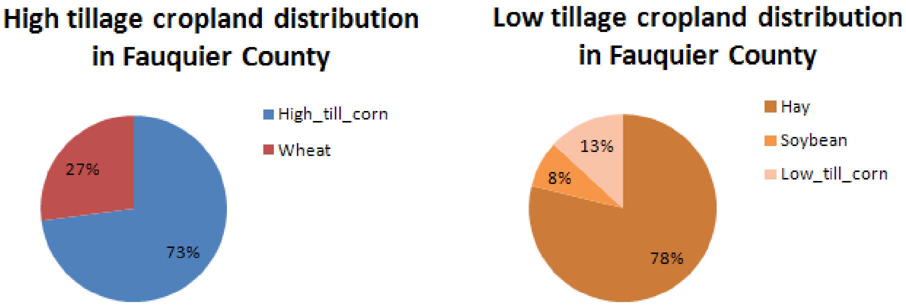


Figure 4-5: High and Low Tillage Cropland Distributions in Fauquier County

Nutrient reactions for the AGCHEM application

The AGCHEM algorithm was originally developed for use on agricultural lands, but can be used on other pervious areas where plant nutrients occur, for example, orchards, nursery land, parks, golf courses, and forests (Bicknell et al., 2005). In this research, the general nitrogen and phosphorus reactions simulated on all pervious areas included: (1) adsorption and desorption of NH_4 (ammonium) and PO_4 (orthophosphate); (2) mineralization of organic nitrogen and phosphorus, and immobilization of NO_3 (nitrate), NH_4 and PO_4; (3) nitrification and denitrification; (4) plant uptake of NO_3, NH_4 and PO_4; and (5) return of plant nitrogen to organic nitrogen. In addition, volatilization of ammonium was simulated on pasture lands, fixation of atmospheric nitrogen was simulated on soybean lands, and detailed organic nitrogen transformations were simulated on forest lands.

Except the adsorption and desorption process and plant uptake for crop lands, other nutrient transformations were generally simulated using first-order kinetics with model parameters of first-order reaction rates and temperature correction factors. The adsorption and desorption process was simulated using Freundlich isotherm method with model parameters including chemical permanently fixed, Freundlich exponent and Freundlich coefficient. The model parameters describing the nutrient reactions were specified in four soil layers separately.

The plant uptake for crop lands was simulated using yield-based method as a function of both soil nutrient level and plant uptake target level. Increasing nutrient application rate would result in increased plant uptake but only up to the target level. Using the yield-based method required input parameters of annual uptake target, monthly fraction of the annual uptake target, and soil layer fraction of the monthly uptake. The annual plant uptake target was estimated by multiplying annual crop yield and nutrient composition in the crop dry weight. Then, the monthly fraction of the annual uptake target was determined based on typical planting and harvesting dates, and crop growth stages in Virginia. Finally, the monthly uptake was distributed among three soil layers including SZ (surface layer), UZ (upper layer) and LZ (lower layer), based on typical crop root depths. The developed input parameters for plant uptake simulation on crop lands were given in Tables 4-2, 4-3 and 4-4. Additionally, nitrogen uptake ratio of NO_3 to NH_4 was specified as 0.8:0.2 in the model.

Table 4-2: Estimated Annual Nutrient Uptake Target for Crop Lands

Crop	Annual yield* (bushel/ac or ton/ac)	Dry weight (lb/bushel)	Nitrogen/phosphorus composition** (%)	Annual nitrogen/phosphorus uptake target (kg/ha)
Corn***	106.0	56	1.6/0.3	107.2/18.6
Wheat	43.7	60	2.1/0.6	61.1/18.3
Soybean	35.3	60	6.3/0.6	148.4/15.2
Hay	2.3		3.0/0.4	150.1/22.2

* An average of the annual crop yields (2002-07) based on USDA National Agricultural Statistics Service (NASS) (USDA, 2004): bushel/ac for corn, wheat and soybean; ton/ac for hay (given in dry weight)

** Average nutrient composition in the crop dry weight based on Agricultural Waste Management Field Handbook (USDA, 1992)

*** Same for high and low tillage corn

Table 4-3: Estimated Monthly Fraction of Annual Nutrient Uptake for Crop Lands

Month	Corn*	Wheat	Soybean	Hay
	Nitrogen/phosphorus uptake (%)	Nitrogen/phosphorus uptake (%)	Nitrogen/phosphorus uptake (%)	Nitrogen/phosphorus uptake (%)
JAN	-	2.5/2.5	-	-
FEB	-	5/5	-	2.5/1.5
MAR	-	10/10	-	2.5/3.5
APR	5/3	30/30	-	11/8.5
MAY	35/17	50/50	-	16.5/14
JUN	33/45	-	5/5	17.5/22.5
JUL	22/28	-	20/20	17.5/22.5
AUG	5/7	-	50/50	16.5/14
SEP	-	-	20/20	11/8.5
OCT	-	-	5/5	2.5/3.5
NOV	-	-	-	2.5/1.5
DEC	-	2.5/2.5	-	-
Total	100/100	100/100	100/100	100/100

* Same for high and low tillage corn

Table 4-4: Estimated Soil Layer Fraction of Monthly Nitrogen and Phosphorus Uptake for Crop Lands

Month	Corn*				Wheat				Soybean				Hay			
	SZ (%)	UZ (%)	LZ (%)	Total (%)	SZ (%)	UZ (%)	LZ (%)	Total (%)	SZ (%)	UZ (%)	LZ (%)	Total (%)	SZ (%)	UZ (%)	LZ (%)	Total (%)
JAN	-	-	-	-	5	30	65	100	-	-	-	-	-	-	-	-
FEB	-	-	-	-	5	30	65	100	-	-	-	-	5	25	70	100
MAR	-	-	-	-	5	30	65	100	-	-	-	-	5	25	70	100
APR	5	95	-	100	5	30	65	100	-	-	-	-	5	25	70	100
MAY	5	45	50	100	5	30	65	100	-	-	-	-	5	25	70	100
JUN	5	30	65	100	-	-	-	-	5	95	-	100	5	25	70	100
JUL	5	60	35	100	-	-	-	-	5	45	50	100	5	25	70	100
AUG	5	60	35	100	-	-	-	-	5	30	65	100	5	25	70	100
SEP	-	-	-	-	-	-	-	-	5	60	35	100	5	25	70	100
OCT	-	-	-	-	-	-	-	-	5	60	35	100	5	25	70	100
NOV	-	-	-	-	-	-	-	-	-	-	-	-	5	25	70	100
DEC	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-

* Same for high and low tillage corn

Nutrient inputs for the AGCHEM application

Nutrient inputs from atmospheric deposition, fertilization and manure application were required for the AGCHEM application. The wet and dry atmospheric depositions of NH_4, NO_3 and PO_4 were input as monthly fluxes into surface soil layer for all land uses. In this research, extensive effort was spent on estimating nutrient inputs from fertilization and manure application.

Manure application

Manure was considered as a common source of soil enrichment for pasture. To estimate the amount of manure input to pasture, livestock population data in Fauquier County from the 2002 Census of Agriculture was used. The livestock included beef, dairy, poultry, swine and sheep. Based on discussions with a nutrient management specialist at Fauquier County DCR (Marshall, 2009), animals like dairy, poultry and swine are kept mostly in confined areas and such areas in the studied watershed were minimal. The beef and sheep were assumed to graze on pasture throughout the year. Since sheep population was minimal compared to beef, manure deposition rates were calculated by dividing the amount of animal waste produced from beef by the acres of pasture. Manure production rates were based on beef excretion estimates from the Agricultural Waste Management Field Handbook (USDA, 1992). For modeling purposes, the manure nitrogen was further split into organic nitrogen and NH_4 with a ratio of 55 to 45 percent, and manure phosphorus was assumed to be 50% organic phosphorus and 50% PO_4 (Kieffer, 2002; Marshall, 2009). Then, the developed nutrient inputs from manure were included as monthly fluxes into the surface soil layer in the forms of NH_4, organic nitrogen, PO_4, and organic phosphorus (Table 4-5).

Table 4-5: Estimated Monthly Manure Nitrogen and Phosphorus Inputs to Pasture

Month	Manure produced (kg/ha)	Manure nitrogen (kg/ha)	Manure phosphorus (kg/ha)	Manure NH_4 input (kg/ha)	Manure organic N input (kg/ha)	Manure PO_4 input (kg/ha)	Manure organic P input (kg/ha)
JAN	559.09	2.91	1.09	1.310	1.600	0.545	0.545
FEB	504.98	2.63	0.98	1.184	1.446	0.490	0.490
MAR	559.09	2.91	1.09	1.310	1.600	0.545	0.545
APR	541.05	2.82	1.05	1.269	1.551	0.525	0.525
MAY	559.09	2.91	1.09	1.310	1.600	0.545	0.545
JUN	541.05	2.82	1.05	1.269	1.551	0.525	0.525
JUL	559.09	2.91	1.09	1.310	1.600	0.545	0.545
AUG	559.09	2.91	1.09	1.310	1.600	0.545	0.545
SEP	541.05	2.82	1.05	1.269	1.551	0.525	0.525
OCT	559.09	2.91	1.09	1.310	1.600	0.545	0.545
NOV	541.05	2.82	1.05	1.269	1.551	0.525	0.525
DEC	559.09	2.91	1.09	1.310	1.600	0.545	0.545
Total	6582.81	34.28	12.81	15.430	18.850	6.405	6.405

Note: Each monthly value was calculated by multiplying daily value and days in the month. The daily manure produced, manure nitrogen and manure phosphorus were 18.035 kg/ha/day, 0.094 kg/ha/day and 0.035 kg/ha/day, respectively.

Fertilization

Commercial fertilizer was considered as an important nutrient source in the study area for almost all other land uses except forest. Generally, one typical fertilizer application was developed separately for each fertilized land use, based on recommendations from the Virginia Nutrient Management Standards and Criteria (VDCR, 2005) and personal discussions with Fauquier county extension agents (Ohlwiler, 2009). The best available data to support the recommendation included Fauquier county crop yields from USDA National Agricultural Statistics Service (NASS) (USDA, 2004) and Fauquier county soil phosphorus test summary from the Virginia Tech Soil Testing Laboratory. The nitrogen application was recommended based on soil productivity group, which was mostly determined by crop yields. The recommended phosphorus application was based on both soil productivity group and soil phosphorus test levels. The estimated fertilizer applications (including application rate, timing and technique) are summarized for each fertilized land use below.

Pasture: 45 kg/ha of N and 28 kg/ha of P_2O_5 were applied in August by surface broadcast on fescue-clover pasture.

Hay: 90 kg/ha of N and 56 kg/ha of P_2O_5 were applied in March by surface broadcast on fescue hay.

Corn: 34 kg/ha of N was applied as a starter fertilizer in April by soil incorporation technique and 101 kg/ha of N was applied in May by surface broadcast; 68 kg/ha of P_2O_5 was applied in April, with half of the application by surface broadcast and the other half by soil incorporation technique.

Wheat: 34 kg/ha of N was applied as a starter fertilizer in September and 78 kg/ha of N was applied in February, all by surface broadcast; 56 kg/ha of P_2O_5 was applied in September by surface broadcast.

Soybean: Nitrogen fertilizer was not required for this leguminous crop; 56 kg/ha of P_2O_5 was applied in May by surface broadcast.

Fertilizer was also applied for mixed cool season tall fescue grass and Kentucky blue grass grown in pervious urban areas, including industrial, institutional, LDR, MDR and townhouse. Fertilizer was applied by surface broadcast, with distribution of 14.5%-28.5%-28.5%-28.5% (sum = 100%) for May-September-October-November. For the pervious areas in industrial and institutional, the annual N and P_2O_5 application rates were 90 kg/ha and 45 kg/ha, respectively. For the pervious areas in LDR, MDR and townhouse, the annual N and P_2O_5 application rates were 78 kg/ha and 34 kg/ha, respectively.
The estimated fertilizer applications were then manipulated for modeling purposes. First, the nutrients were required to be in one of the following specific forms: NO_3, NH_4, organic nitrogen, PO_4, and organic phosphorus. For simplification, 25% of N application was assumed to be converted into NO_3, 75% of N application was assumed to be

converted into NH_4, and 100% of P_2O_5 application was assumed to be converted into PO_4. Second, the nutrient inputs were required to be applied to either the surface or the upper soil layer. This depended on the recommended nutrient application technique. With surface broadcast, fertilizer was applied to the surface layer. With the soil incorporation technique, 10% of the fertilizer was applied to the surface layer and the remaining 90% was incorporated into the upper layer based on the assumption that incorporation would produce an approximately uniform distribution of nutrient in the top two soil layers (Donigian et al., 1994). The developed NH_4, NO_3 and PO_4 inputs from fertilizer for each fertilized land use were included as monthly fluxes into surface soil layer (SZ) and upper soil layer (UZ), as shown in Table 4-6.

Table 4-6: Estimated NH_4, NO_3 and PO_4 Inputs for Fertilized Land Uses (kg/ha)

Month	Pasture		Hay		Corn**		Wheat		Soybean		Industrial/ Institutional		LDR /MDR/ Townhouse	
	SZ	UZ	SZ	UZ	SZ	UZ	SZ	UZ	SZ	UZ	SZ	UZ	SZ	UZ
JAN	-	-	-	-	-	-	-	-	-	-	-	-	-	-
FEB	-	-	-	-	-	-	58.9* (19.6/-)	-	-	-	-	-	-	-
MAR	-	-	67.3* (22.4/24.4)	-	-	-	-	-	-	-	-	-	-	-
APR	-	-	-	-	2.6* (0.9/16.1)	22.6* (7.5/13.2)	-	-	-	-	-	-	-	-
MAY	-	-	-	-	75.7* (25.2/-)	-	-	-	-* (-	-	9.8* (3.3/2.8)	-	8.4* (2.8/2.2)	-
JUN	-	-	-	-	-	-	-	-	-	-	-	-	-	-
JUL	-	-	-	-	-	-	-	-	-	-	-	-	-	-
AUG	33.6* (11.2/12.3)	-	-	-	-	-	-	-	-	-	-	-	-	-
SEP	-	-	-	-	-	-	25.2* (8.4/24.4)	-	-	-	19.2* (6.4/5.6)	-	16.8* (5.6/4.1)	-
OCT	-	-	-	-	-	-	-	-	-	-	19.2* (6.4/5.6)	-	16.8* (5.6/4.1)	-
NOV	-	-	-	-	-	-	-	-	-	-	19.2* (6.4/5.6)	-	16.8* (5.6/4.1)	-
DEC	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	33.6* (11.2/12.3)		67.3* (22.4/24.4)		100.9* (33.6/29.3)		84.1* (28/24.4)		- * (-/24.4)		67.4* (22.5/19.6)		58.8* (19.6/14.5)	

* Values outside of ( ) are NH_4 inputs; Values in ( ) are NO_3 and PO_4 inputs

** Same for high and low tillage corn

4.3.3 Model Calibration and Validation

The HSPF with PQUAL application by Liu et al. (2011a) was calibrated from 2002 to 2005 and validated from 2006 to 2007 using observed data from the stream station ST70. It was considered to provide a very good representation of flow and a reasonable good representation of sediment loading.

With the same flow and sediment calibration as the previous HSPF application, this research focused on adjusting AGCHEM parameters to obtain a satisfactory agreement between simulated and observed OP (orthophosphate phosphorus) loading, NH_4-N (ammonium nitrogen) loading and Ox-N (oxidized nitrogen) loading. Parameter selection and value ranges for the calibration were based on the literature values (for example, Donigian et al., 1999; Kieffer, 2002). Information from local studies and preliminary sensitivity analysis also helped with the calibration process.

The agreement between simulated and observed nutrient loadings was evaluated by visual and statistical comparisons on annual, seasonal and monthly scales during calibration and validation periods. The statistical comparisons are presented with percentage difference (PD) and the standard coefficient of determination (R^2). The percentage difference (PD) between simulated and observed data is defined as

$$PD = \frac{100 \cdot (Y - X)}{X}\% \qquad (1)$$

Where X is the observed value, and Y is the simulated value.

4.3.4 Sensitivity Analysis

“One-variable-at-a-time” sensitivity analysis was performed to examine the sensitivity of nutrient loadings with respect to model input parameters, including: meteorological inputs, nutrient inputs (atmospheric, manure and fertilizer application rates, and fertilizer application time) and parameters related to streamflow generation, sediment and nutrient transport and interactions on lands and within streams. The sensitivity analysis was performed for the calibrated model based on both average yearly and average seasonal (spring, summer, fall, winter) values of the nutrient loadings.

Except for fertilizer application time, sensitivity results are displayed with normalized sensitivity index (*S*). The normalized sensitivity index (*S*) was calculated as

$$S = \frac{\Delta y / y}{\Delta x / x} = \frac{(y_2 - y_1)/y}{(x_2 - x_1)/x} \qquad (2)$$

Where x is the base value of parameter, y is the base value of output, and x_2 and x_1 indicate a ±10% change of the parameter values, respectively. Correspondingly, y_2 and y_1 indicate the output responses to x_2 and x_1. *S* can be positive, zero or negative indicating positive correlation, no correlation, and negative correlation. The greater the absolute value, the more sensitive a model output is to a particular parameter (White and Chaubey, 2005).

The sensitivity analysis for fertilizer application time was conducted by a series of "sensitivity scenarios": assume an alternate fertilizer application time and redevelop related nutrient inputs, then run the model to examine the percentage change of nutrient loading. The sensitivity result represented with the percentage change (*SPD*) was calculated as

$$SPD = \frac{100 \cdot (y_1 - y)}{y} \% \qquad (3)$$

Where y is the nutrient loading from the base scenario, and y_1 is the nutrient loading generate from the alternate fertilizer application time.

4.4 Results and Discussion

4.4.1 Model Calibration and Validation Results

The simulated OP, Ox-N and NH_4-N loadings were compared with their observed values based on annual, seasonal and monthly scales during calibration and validation periods, as shown in Tables 4-7, 4-8 and 4-9, respectively.

OP calibration was considered to be good overall. Over the four-year calibration period, the total OP loading was underestimated by 11.2% (Table 4-7). The relatively large PD value in the wet year 2003 (–25.9%, Table 4-7) was mainly due to under prediction of OP loading in June when there were intense storms, which might also help to explain the relatively large error of predicting summer average OP loading (–46.2%, Table 4-8) during the calibration period. The low PD values in other seasons (from –16.8% to +14.6%, Table 4-8) and high R^2 value based on monthly comparison (0.818, Table 4-9) indicated that temporal variation of OP loading was captured well.

The annual Ox-N and NH_4-N loadings were also predicted well during the calibration period. The total Ox-N and NH_4-N loadings from 2002 to 2005 were underestimated by 8% and 3.2% (Table 4-7). The PD values of the annual Ox-N and NH_4-N loadings for most years were within ±15%. As shown in Table 4-7, the exceptions occurred in 2002 with PD values of +21.5% and –34.8% for Ox-N and NH_4-N loading respectively. Because the annual Ox-N and NH_4-N loadings in the year 2002 were small compared to other years (Table 4-7), these had limited impact overall. The temporal variation of Ox-N loading was captured reasonably well. Comparatively, the temporal variation of NH_4-N loading was not captured as well, indicated by relatively large PD values based on seasonal comparisons (from –88.3% to +38.3%, Table 4-8) and relatively low R^2 value based on monthly comparisons (0.270, Table 4-9).

As expected, the nutrient validation results showed generally weaker correlations between observed and simulated data than the calibration results, based on annual and seasonal comparisons as indicated by PD (Tables 4-7 and 4-8) and monthly comparison as indicated by R^2 (Table 4-9). Overall, the model performance for OP validation was better than Ox-N and NH_4-N validation. The Ox-N loading was generally over-predicted, and the NH_4-N loading was generally under-predicted, especially in summer and fall.

Table 4-7: Annual Comparison by Variable and Year during Calibration and Validation Periods for the HSPF/AGCHEM Application

	Calibration					Validation		
	2002	2003	2004	2005	Total (2002-2005)	2006	2007	Total (2006-2007)
OP (10^6 g)	–20.5%	–25.9%	+7.3%	+8.3%	–11.2%	–33.5%	–13.6%	–25.7%
	(0.31/0.25)	(1.78/1.32)	(0.69/0.74)	(0.85/0.92)	(3.63/3.23)	(0.94/0.62)	(0.60/0.52)	(1.54/1.14)
Ox-N (10^6 g)	+21.5%	–15.6%	–14.1%	–2.5%	–8.0%	+18.4%	+34.8%	+24.2%
	(18.23/22.15)	(70.27/59.32)	(34.05/29.25)	(37.14/36.21)	(159.69/146.93)	(25.24/29.87)	(13.99/18.85)	(39.23/48.72)
NH_4-N (10^6 g)	–34.8%	+4.9%	–13.1%	+5.8%	–3.2%	–49.1%	+63.5%	–17.5%
	(1.34/0.87)	(5.38/5.64)	(2.29/1.99)	(2.43/2.57)	(11.44/11.07)	(1.58/0.80)	(0.62/1.01)	(2.20/1.81)

Note: Values in ( ) below PD values are the observed and simulated loads

Table 4-8: Seasonal Average Comparison by Variable during Calibration and Validation Periods for the HSPF/AGCHEM Application

		Spring (March – May)	Summer (June – August)	Fall (September – November)	Winter (December – February)
OP (10^6 g)	Calibration (2002-2005)	+14.6%	–46.2%	–11.6%	–16.8%
		(0.31/0.35)	(0.19/0.10)	(0.20/0.18)	(0.21/0.18)
	Validation (2006-2007)	–9.4%	–7.1%	–42.4%	–24.0%
		(0.24/0.22)	(0.06/0.06)	(0.32/0.19)	(0.15/0.11)
Ox-N (10^6 g)	Calibration (2002-2005)	+20.2%	–9.9%	+15.7%	–47.5%
		(12.83/15.43)	(6.11/5.50)	(7.56/8.75)	(13.42/7.05)
	Validation (2006-2007)	+20.3%	+149.1%	+98.2%	–33.3%
		(5.21/6.27)	(1.74/4.34)	(4.03/8.00)	(8.63/5.76)
NH_4-N (10^6 g)	Calibration (2002-2005)	+16.5%	–88.3%	–2.1%	+38.3%
		(1.21/1.41)	(0.63/0.07)	(0.32/0.31)	(0.71/0.98)
	Validation (2006-2007)	+25.3%	–94.3%	–43.1%	+52.6%
		(0.33/0.41)	(0.26/0.01)	(0.31/0.18)	(0.20/0.30)

Note: Values in ( ) below PD values are the observed and simulated loads

Table 4-9: Monthly R^2 by Variable during Calibration and Validation Periods for the HSPF/AGCHEM Application

	OP	Ox-N	NH_4-N
Calibration (2002-2005)	0.818	0.407	0.270
Validation (2006-2007)	0.430	0.305	0.177

A close investigation was performed on the calibrated model for simulated nutrient balance on each land use. Table 4-10 shows the nutrient inputs and outputs for main fertilized land types, with the difference between inputs and outputs as nutrient storage in the soil. The primary phosphorus input was PO_4 application from fertilizer and manure (14.5 to 29.3 kg/ha/yr). Other phosphorus inputs included atmospheric deposition of PO_4 and organic P application from manure on pasture. The primary phosphorus output was by plant uptake (12.7 to 31.1 kg/ha/yr). The PO_4 loss could also be associated with surface runoff and subsurface flow. For every fertilized land types, the primary nitrogen input was NH_4 and NO_3 application from fertilizer and manure (49.1 to 100.9 kg/ha/yr for NH_4 and 11.2 to 33.6 kg/ha/yr for NO_3), and the primary nitrogen output was by plant uptake (44.1 to 70.1 kg/ha/yr). Similar to the phosphorus balance, the nitrogen balance also accounted for inputs from atmospheric deposition of NH_4 and NO_3 as well as organic N application from manure on pasture. Denitrification and volatilization (specially on pasture) were considered as nutrient outputs in the nitrogen balance. Other outputs for the nitrogen balance included NH_4 and NO_3 loss associated with surface runoff and subsurface flow. Compared to PO_4 and NH_4, NO_3 is easier to leach and transport with subsurface flow (Hantzsche and Finnemore, 1991). In addition, agricultural lands (for example, hay, high and low tillage corn, and wheat) seemed to contribute more of the nutrient loadings from the watershed.

Table 4-10: Simulated Nutrient Balance for Main Fertilized Land Types

	Pasture	Hay	High tillage corn	Low tillage corn	Wheat	Industrial/ Institutional	Low density residential
			Phosphorus balance (kg/ha/yr)				
Inputs	**24.6**	**24.5**	**29.4**	**29.4**	**24.5**	**19.7**	**14.6**
PO_4 application from fertilizer and manure	18.4	24.4	29.3	29.3	24.4	19.6	14.5
Organic P application from manure	6.1	0.0	0.0	0.0	0.0	0.0	0.0
Atmos. deposition of PO_4	0.1	0.1	0.1	0.1	0.1	0.1	0.1
Outputs	**31.3**	**31.5**	**29.9**	**30.0**	**18.2**	**19.9**	**13.0**
Plant uptake of phosphorus	31.1	30.8	29.3	29.6	18.0	19.4	12.7
PO_4 loss with surface runoff	0.1	0.4	0.3	0.2	0.1	0.3	0.2
PO_4 loss with leaching & subsurface Flow	0.1	0.3	0.3	0.2	0.1	0.2	0.1
			Nitrogen balance (kg/ha/yr)				
Inputs	**80.1**	**90.4**	**135.2**	**135.2**	**112.8**	**90.6**	**79.1**
NH_4 application from fertilizer and manure	49.1	67.3	100.9	100.9	84.1	67.4	58.8
NO_3 application from fertilizer and manure	11.2	22.4	33.6	33.6	28.0	22.5	19.6
Organic N application from manure	19.1	0.0	0.0	0.0	0.0	0.0	0.0
Atmos. deposition of NH_4	0.3	0.3	0.3	0.3	0.3	0.3	0.3
Atmos. deposition of NO_3	0.4	0.4	0.4	0.4	0.4	0.4	0.4
Outputs	**56.7**	**80.8**	**117.7**	**103.6**	**105.7**	**81.8**	**72.1**
Plant uptake of nitrogen	47.3	51.5	67.3	67.6	44.1	70.1	61.8
Denitrification &	5.1	2.7	8.9	8.7	8.8	0.7	0.6
NH_4 loss with surface runoff	0.5	3.4	0.8	0.6	4.3	1.0	0.9
NH_4 loss with leaching & subsurface runoff	0.5	3.3	0.8	0.5	4.0	1.0	0.9
NO_3 loss with surface runoff	1.7	8.1	12.8	8.6	9.5	6.2	5.4
NO_3 loss with leaching & subsurface flow	1.6	11.8	27.1	17.6	35.0	2.8	2.5

4.4.2 Sensitivity Analysis Results

The normalized sensitivity index (*S*) was calculated using Equation (2) on 7 meteorological inputs, 3 nutrient inputs (atmospheric, manure and fertilizer application rates), and totally 103 PERLND and REACH parameters for OP loading, Ox-N loading and NH_4-N loading. These inputs and parameters are listed in Table 4-11. The determination of the inputs and parameters involved in the sensitivity analysis was based on literature and experience with HSPF. For each parameter, the calibrated value was used as the base value. The sensitivity analysis for each input/parameter involved two model runs: changing the input/parameter from the base value by +10% (except AGWRC, which was changed to its maximum value of 0.999) and by –10%.

Of the inputs and parameters that were analyzed, only a subset had noticeable impact on model outputs. Table 4-12 shows the subset of inputs and parameters with *S* greater than 0.1 for average annual OP loading, Ox-N loading and NH_4-N loading, organized by four categories: meteorological inputs, nutrient inputs, PERLND parameters and REACH parameters. Some of the PERLND parameters are related to flow generation process and others are related to nitrogen and phosphorus cycle in the soil profile. The inputs and parameters with *S* greater than 0.5 were considered to be significant. That is, a total change of 20% (± 10%) in input/parameter produces a change of 10% or more in model output.

Table 4-12 also displays the sensitivity results represented with percentage change (*SPD*) of nutrient (OP, Ox-N, NH_4-N) loadings on fertilizer application time. The *SPD* was calculated using Equation (3) for three “sensitivity scenarios”, including: (1) fertilizer evenly distributed throughout year; (2) fertilizer applied totally at plant date; and (3) fertilizer evenly distributed between plant and harvest date.

Figures 4-6, 4-7 and 4-8 show sensitivity index (*S*) for average seasonal (spring, summer, fall, winter) OP loading, NH_4-N loading, and Ox-N loading respectively. In each of the figures, only inputs and parameters with *S* greater than 0.5 for any of the seasonal average outputs are shown. In addition, sensitivity of average seasonal nutrient (OP, NH_4-N, Ox-N) loadings to fertilizer application time is displayed as percentage change (*SPD*) in Tables 4-13, 4-14 and 4-15.

Table 4-11: Meteorological Inputs, Nutrient Inputs and HSPF/AGCHEM Parameters Included in the Sensitivity Analysis

Parameter	Description	Parameter	Description
	Meteorological inputs		**PERLND parameters (continued)**
PREC	Precipitation	LZSN	Lower zone nominal storage
ATEM	Air temperature	UZSN	Upper zone nominal storage
DEWP	Dew point temperature	LZETP	Lower zone ET parameter
WIND	Wind speed	DEEPFR	Fraction of ground inflow which enters deep groundwater
SOLR	Solar radiation	JRER	Exponent in the soil detachment equation
CLOU	Cloud cover	KRER	Coefficient in the soil detachment equation
EVAP	Potential evaporation	JSER	Exponent in the detached sediment washoff equation
	Nutrient inputs	KSER	Coefficient in the detached sediment washoff equation
ATM	Atmosphere input	XFIX-P (s, u, l, g)*	Maximum phosphorus concentration permanently fixed to the soil
MAN-R	Manure application rate	K1-P (s, u, l, g)*	Coefficient for phosphorus Freundlich adsorption and desorption equation
FER-R	Fertilizer application rate	KMP (s, u, l, g)*	Organic P mineralization rate
FER-D	Fertilizer application time	KIMP (s, u, l, g)*	Phosphate immobilization rate
	REACH parameters	PHOSUPT (s, u, l,	Plant phosphorus uptake rate
KSAND	Coefficient in the sandload power function formula	PUPTGT	Total annual target for plant uptake of phosphorus
EXPSND	Exponent in the sandload power function formula	XFIX-N (s, u, l, g)*	Maximum ammonium concentration permanently fixed to the soil
TAUCS (silt, clay)	Critical bed shear stress for (silt, clay) scour	K1-N (s, u, l, g)*	Coefficient for ammonium Freundlich adsorption and desorption equation
M (silt, clay)	Erodibility coefficient of (silt, clay)	KAM (s, u, l, g)*	Organic N ammonification rate
TAUCD (silt, clay)	Critical bed shear stress for (silt, clay) deposition	KIMAM (s, u, l, g)*	Ammonium immobilization rate
KTAM20	Nitrification rate of ammonium at 20 ℃	KIMNI (s, u, l, g)*	Nitrate immobilization rate
KNO320	Nitrate denitrification rate at 20 ℃	NITUPT (s, u, l, g)*	Plant nitrogen uptake rate
KBOD20	BOD decay rate at 20 ℃	NUPTGT	Total annual target for plant uptake of nitrogen
ADNHPM (sand, silt, clay)	Adsorption coefficients for NH$_4$ adsorbed to (sand, silt, clay)	KNI (s, u, l, g)*	Nitrification rate
ADPOPM (sand, silt, clay)	Adsorption coefficients for OP adsorbed to (sand, silt, clay)	KDNI (s, u, l, g)*	Denitrification rate
	PERLND parameters	P4AD (s, u, l, g)*	Initial storage of adsorbed phosphate
AGWRC	Base groundwater recession rate	P4SU (s, u, l, g)*	Initial storage of solution phosphate
INFILT	Index to the infiltration capacity of the soil	AMAD (s, u, l, g)*	Initial storage of adsorbed ammonium
INTFW	Interflow inflow parameter	AMSU (s, u, l, g)*	Initial storage of solution ammonium
IRC	Interflow recession parameter	NO$_3$ (s, u, l, g)*	Initial storage of nitrate

*Different parameters for 4 soil layers (s: surface layer; u: upper layer; l: lower layer; g: groundwater layer)

Table 4-12: Sensitivity Index (*S*) of Average Annual Output Variables to HSPF/AGCHEM Inputs and Parameters

Parameter	Description	Calibrated value	OP	Ox-N	NH_4
	Meteorological inputs				
PREC	Precipitation	Not applicable	+2.6	+1.2	+2.3
ATEM	Air temperature	Not applicable	–1.2	–0.5	–1.8
EVAP	Potential Evaporation	Not applicable	–0.7	–0.3	–0.5
DEWP	Dew point temperature	Not applicable			–0.1
	Nutrient inputs				
FER-R	Fertilizer application rate	Not applicable	+0.7	+1.2	+0.5
MAN-R	Manure application rate	Not applicable	+0.3	+0.1	+0.4
FER-D1*	Fertilizer evenly distributed throughout year	Not applicable	+24.3%		+36.8%
FER-D2*	Fertilizer applied totally at plant date	Not applicable	+22.4%	+10.5%	+14.8%
FER-D3*	Fertilizer evenly distributed between plant and harvest date	Not applicable	+10.4%		–16.7%
	PERLND parameters				
AGWRC	Base groundwater recession rate	0.92	–0.2	–2.9	–0.8
LZETP	Lower zone ET parameter	0.46-0.6***	–0.5	–0.2	–0.2
LZSN	Lower zone nominal storage	5	–0.2	–0.4	–0.4
UZSN	Upper zone nominal storage	0.4-0.62***	–0.7	–0.2	–0.6
INFILT	Index to the infiltration capacity of the soil	0.13-0.18**	–0.8	–0.2	–0.7
INTFW	Interflow inflow parameter	3	–0.3		
XFIX-P(u)	Maximum phosphorus concentration permanently fixed to the soil (upper layer)	40	–0.3		
K1-P(s)	Coefficient for phosphorus Freundlich adsorption and desorption equation (surface layer)	6	+0.2		
NUPTGT	Total annual target for plant uptake of nitrogen	54.5-133.9**		–0.5	
AMAD(g)	Initial storage of adsorbed ammonium (groundwater layer)	5-7**		+0.3	+1.0
XFIX-N(g)	Maximum concentration of ammonium permanently fixed to the soil (groundwater layer)	0.3		–0.3	–0.9
KNI(u)	Nitrification rate (upper layer)	50			–0.3
K1-N(u)	Coefficient for ammonium Freundlich adsorption and desorption equation (upper layer)	1			–0.1
	REACH parameters				
KTAM20	Nitrification rate of ammonia at 20 ℃	0.05	–0.1		–0.3

* Sensitivity result based on “sensitivity scenarios” is presented as *SPD* (%)

** Varying by land use

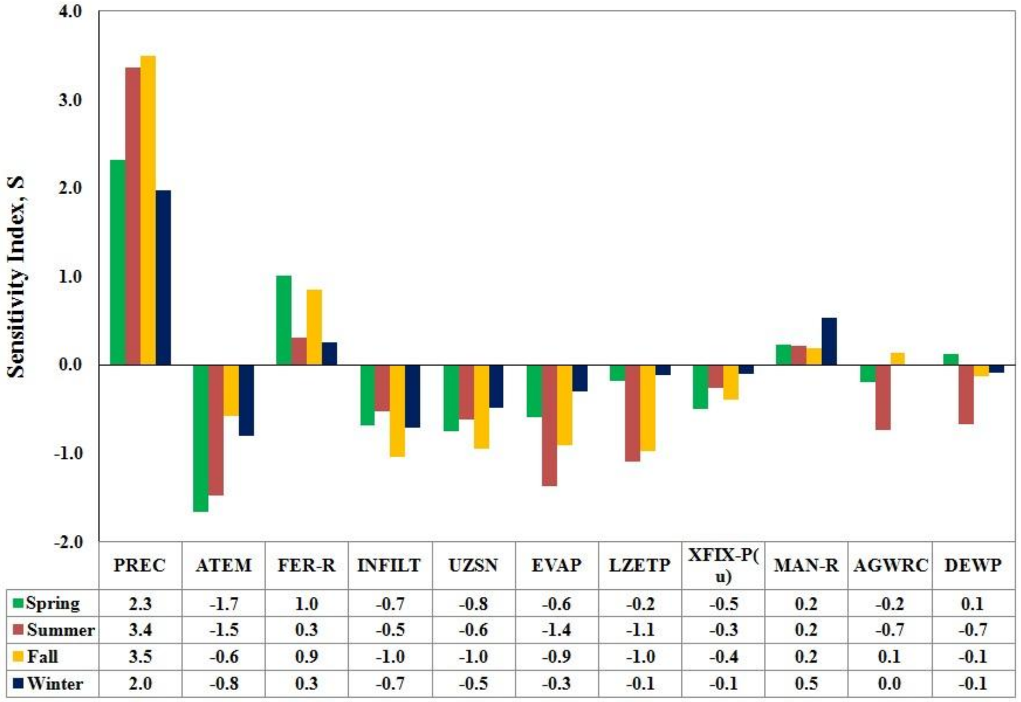
*** Varying by month and land use

OP sensitivity analysis

As shown in Table 4-12, the average annual OP loading was significantly impacted by meteorological inputs, especially precipitation, which had an *S* value of +2.6. Several important parameters describing the flow generation process had significant impact on the average annual OP loading, including INFILT (index to the infiltration capacity of the soil), UZSN (upper zone nominal storage) and LZETP (lower zone ET parameter). INFILT, UZSN and LZETP were all negatively correlated with the average annual OP loading.

As the primary nutrient input, fertilizer application was quite important for OP simulation. The average annual OP loading was positively correlated with the fertilizer application rate (*S*=+0.7, Table 4-12). Fertilizer application time also had significant impact on the average annual OP loading. As shown in Table 4-12, FER-D1 (fertilizer evenly distributed throughout year) and FER-D2 (fertilizer applied totally at plant date) caused more than 20% increase of the average annual OP loading. Of the AGCHEM parameters, XFIX-P (maximum phosphorus concentration permanently fixed to the soil) describing phosphorus adsorption and desorption in upper soil layer was relatively more important.

Figure 4-6 shows sensitivity results for average seasonal OP loadings, similar to the annual sensitivity analysis, except a little more significant impact of certain input parameters in certain season. For example, the relatively higher *S* values of PREC, EVAP and LZETP in summer was probably due to the flow generation associated with intense storm events and higher ET during the season. As shown in Table 4-13, changing fertilizer application time showed significantly different seasonal impacts. Among the three "sensitivity scenarios", FER-D3 (fertilizer evenly distributed between plant and harvest date) had relatively small impacts overall. As expected for FER-D2, when fertilizer was totally applied at plant date, the spring average OP loading greatly increased (*SPD*=+71.1%, Table 4-13). Since plant growth and OP uptake was limited at winter, FER-D1 (fertilizer evenly distributed throughout year) caused a great increase of average winter OP loading (*SPD*=+90.6%, Table 4-13).



	PREC	ATEM	FER-R	INFILT	UZSN	EVAP	LZETP	XFIX-P(u)	MAN-R	AGWRC	DEWP
🟩 Spring	2.3	-1.7	1.0	-0.7	-0.8	-0.6	-0.2	-0.5	0.2	-0.2	0.1
🟥 Summer	3.4	-1.5	0.3	-0.5	-0.6	-1.4	-1.1	-0.3	0.2	-0.7	-0.7
🟨 Fall	3.5	-0.6	0.9	-1.0	-1.0	-0.9	-1.0	-0.4	0.2	0.1	-0.1
🟦 Winter	2.0	-0.8	0.3	-0.7	-0.5	-0.3	-0.1	-0.1	0.5	0.0	-0.1

Figure 4-6: Sensitivity Index (*S*) of Average Seasonal OP Loading to HSPF/AGCHEM Inputs and Parameters

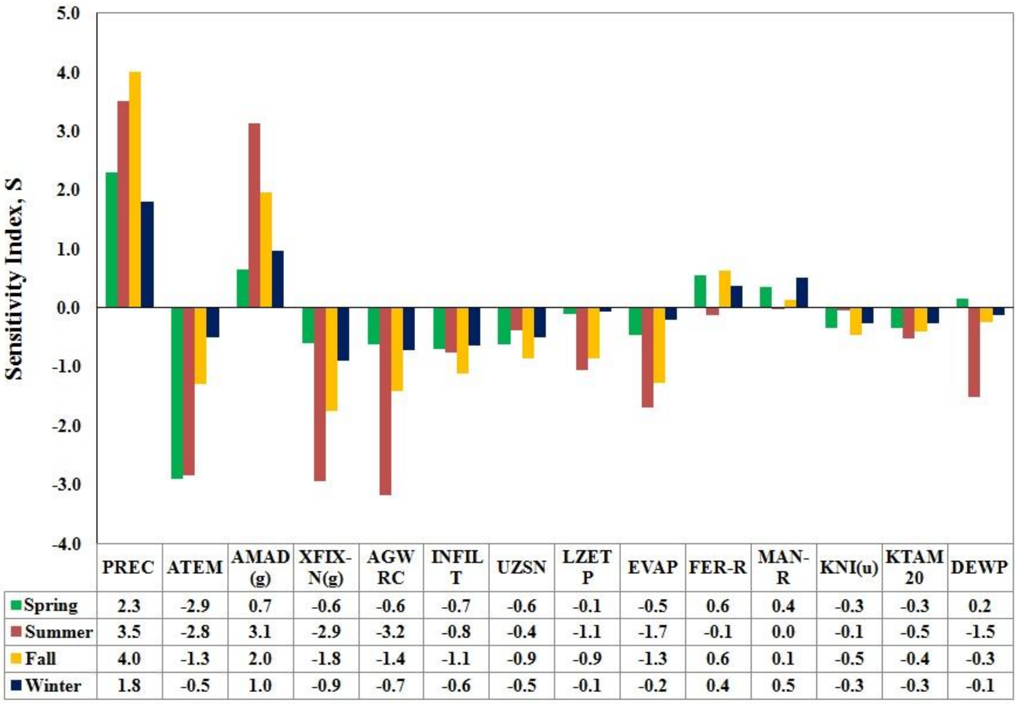
Table 4-13: Sensitivity of Average Seasonal OP Loading to Fertilizer Application Time (as Percentage Change *SPD*)

	Spring	Summer	Fall	Winter
FER-D1 (Fertilizer evenly distributed throughout year)	+0.6%	+33.6%	–0.3%	+90.6%
FER-D2 (Fertilizer applied totally at plant date)	+71.1%	+11.0%	–35.1%	–9.8%
FER-D3 (Fertilizer evenly distributed between plant and harvest date)	–11.6%	+54.2%	+18.5%	+20.3%

NH_4-N sensitivity analysis

As shown in Table 4-12, meteorological inputs (including precipitation, air temperature and potential evaporation) significantly impact flow generation and thus play an important role in NH_4-N load generation. The PERLND parameters closely related to the flow process also had significant impact on the average annual NH_4-N loading, for example, INFILT, UZSN and AGWRC (base groundwater recession rate). The NH_4-N load generation was quite sensitive to AGCHEM parameters describing nitrogen cycle in the soil. Among the AGCHEM parameters, AMAD (initial storage of absorbed ammonium, *S*=+1.0, Table 4-12) and XFIX-N (maximum concentration of ammonium permanently fixed to the soil, *S*=–0.9, Table 4-12) describing ammonium adsorption and desorption in groundwater layer were most significant. In addition, the average annual NH_4-N loading was negatively correlated with nitrification rate (KNI) in upper layer. Figure 4-7 shows sensitivity results for average seasonal NH_4-N loadings, similar to the annual sensitivity analysis. Most sensitive inputs and parameters became a little more significant in summer.

The average annual NH_4-N loading was positively correlated with the fertilizer application rate (*S*=+0.5, Table 4-12). Fertilizer application time also had significant impact on the average annual NH_4-N loading. As shown in Table 4-12, FER-D1 (fertilizer evenly distributed throughout year) caused 36.8% increase of the average annual NH_4-N loading. As for OP, FER-D2 (fertilizer applied totally at plant date) greatly increased the spring average NH_4-N loading (*SPD*=+61.6%, Table 4-14). FER-D1 (fertilizer evenly distributed throughout year) caused a great increase of average winter NH_4-N loading (*SPD*=+80.8%, Table 4-14).



	PREC	ATEM	AMAD (g)	XFIX-N(g)	AGW RC	INFIL T	UZSN	LZET P	EVAP	FER-R	MAN-R	KNI(u)	KTAM 20	DEWP
🟩 Spring	2.3	-2.9	0.7	-0.6	-0.6	-0.7	-0.6	-0.1	-0.5	0.6	0.4	-0.3	-0.3	0.2
🟥 Summer	3.5	-2.8	3.1	-2.9	-3.2	-0.8	-0.4	-1.1	-1.7	-0.1	0.0	-0.1	-0.5	-1.5
🟨 Fall	4.0	-1.3	2.0	-1.8	-1.4	-1.1	-0.9	-0.9	-1.3	0.6	0.1	-0.5	-0.4	-0.3
🟦 Winter	1.8	-0.5	1.0	-0.9	-0.7	-0.6	-0.5	-0.1	-0.2	0.4	0.5	-0.3	-0.3	-0.1

Figure 4-7: Sensitivity Index (*S*) of Average Seasonal NH_4-N Loading to HSPF/AGCHEM Inputs and Parameters

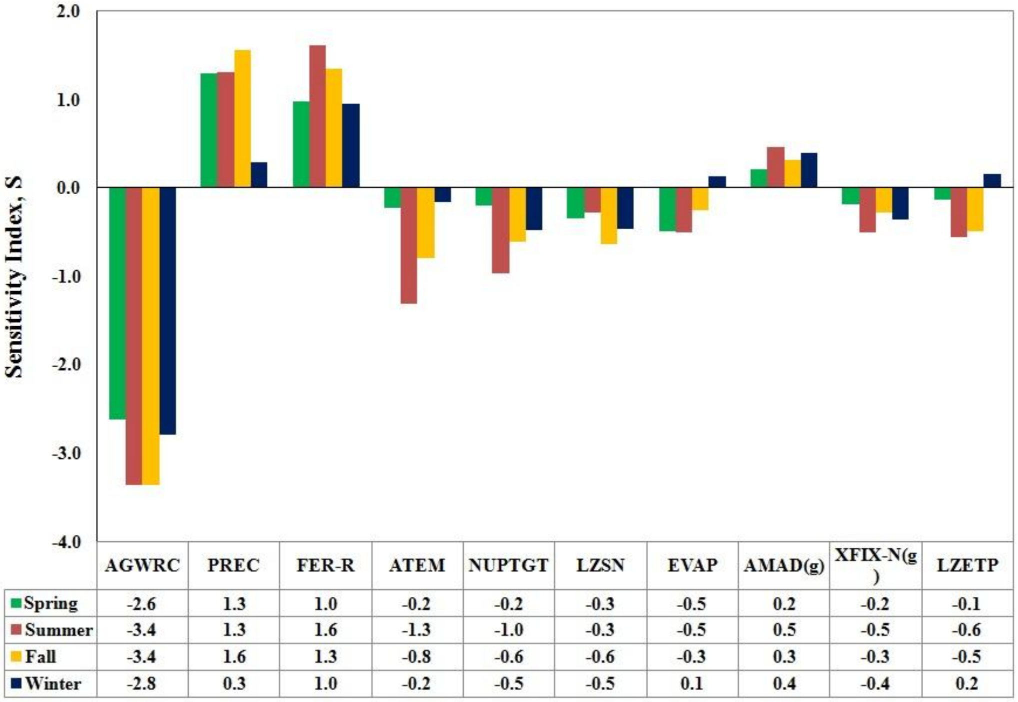
Table 4-14: Sensitivity of Average Seasonal NH_4-N Loading to Fertilizer Application Time (as Percentage Change *SPD*)

	Spring	Summer	Fall	Winter
FER-D1 (Fertilizer evenly distributed throughout year)	+19.6%	+9.9%	–17.3%	+80.8%
FER-D2 (Fertilizer applied totally at plant date)	+61.6%	–13.4%	–52.2%	–29.7%
FER-D3 (Fertilizer evenly distributed between plant and harvest date)	–24.0%	+11.9%	–9.7%	–10.5%

Ox-N sensitivity analysis

Although the average annual Ox-N loading was significantly impacted by precipitation (*S*=+1.2, Table 4-12), the most sensitive parameter was AGWRC (*S*=–2.9, Table 4-12), the key parameter to impact groundwater discharge. Possibly this was because NO_3 was easier to leach and transport with subsurface flow, as discussed earlier. Among the AGCHEM parameters describing nitrogen cycle in the soil, the average annual Ox-N loading was most sensitive to NUPTGT (total annual target for plant uptake of nitrogen, *S*=–0.5 in Table 4-12). As shown in Figure 4-8, these sensitive parameters were found to have similar impacts for average seasonal Ox-N loadings.

Fertilizer application rate was very important for Ox-N load generation. The average annual Ox-N loading was positively correlated with the fertilizer application rate (*S*=+1.2, Table 4-12). As seen in Tables 4-12 and 4-15, compared to OP and NH_4-N, the Ox-N loadings were less impacted by fertilizer application time.



	AGWRC	PREC	FER-R	ATEM	NUPTGT	LZSN	EVAP	AMAD(g)	XFIX-N(g)	LZETP
🟩 **Spring**	-2.6	1.3	1.0	-0.2	-0.2	-0.3	-0.5	0.2	-0.2	-0.1
🟥 **Summer**	-3.4	1.3	1.6	-1.3	-1.0	-0.3	-0.5	0.5	-0.5	-0.6
🟨 **Fall**	-3.4	1.6	1.3	-0.8	-0.6	-0.6	-0.3	0.3	-0.3	-0.5
🟦 **Winter**	-2.8	0.3	1.0	-0.2	-0.5	-0.5	0.1	0.4	-0.4	0.2

Figure 4-8: Sensitivity Index (*S*) of Average Seasonal Ox-N Loading to HSPF/AGCHEM Inputs and Parameters

Table 4-15: Sensitivity of Average Seasonal Ox-N Loading to Fertilizer Application Time (as Percentage Change *SPD*)

	Spring	Summer	Fall	Winter
FER-D1 (Fertilizer evenly distributed throughout year)	–0.5%	–47.6%	–13.3%	+38.9%
FER-D2 (Fertilizer applied totally at plant date)	+52.2%	+14.7%	–31.3%	–32.3%
FER-D3 (Fertilizer evenly distributed between plant and harvest date)	–27.8%	–39.4%	+15.6%	+26.3%

4.5 Conclusions

The nutrient algorithm AGCHEM was used in the HSPF model for the Upper Broad Run watershed. Extensive effort was spent on estimating fertilizer and manure related nutrient inputs for the AGCHEM application. Generally, one typical fertilizer application throughout the watershed during the entire simulation period was developed separately for each fertilized land use, based on recommendations from the Virginia Nutrient Management Standards and Criteria (VDCR, 2005) and personal discussions with Fauquier county extension agents (Ohlwiler, 2009).

The model was considered to provide a reasonable good representation of nutrient loadings, based on annual, seasonal and monthly comparisons during the four-year calibration period (2002-2005) and two-year validation period (2006-2007). A close investigation was performed on the calibrated model for nitrogen and phosphorus balance for main fertilized land types. The primary nutrient input was PO_4, NH_4 and NO_3 application from fertilizer and manure. The primary nutrient output was by plant uptake. Compared to PO_4 and NH_4, NO_3 was easier to leach and transport with subsurface flow.

“One-variable-at-a-time” sensitivity analysis was performed on the calibrated model to examine the sensitivity of nutrient loadings with respect to model inputs and parameters, including: meteorological inputs, nutrient inputs (atmospheric, manure, fertilizer application rates, and fertilizer application time), PERLND parameters related to flow generation and nutrient reactions in the soil, and REACH parameters describing chemical and biological processes within streams. Except for fertilizer application time, sensitivity results were displayed with normalized sensitivity index (*S*). The sensitivity analysis for fertilizer application time was conducted based on three “sensitivity scenarios” and the sensitivity results were represented with percentage change (*SPD*) of nutrient loadings.

Generally, all the nutrient loadings were quite sensitive to meteorological inputs, especially precipitation, indicating the importance of accurately representing climate conditions for the watershed. As the primary nutrient input, fertilizer application was found to be very important for the nutrient load generation. The nutrient loadings were positively correlated with the fertilizer application rate. Changing fertilizer application time showed significant impacts on seasonal nutrient loadings.

Of the AGCHEM parameters describing nitrogen cycle in the soil, the NH_4-N load generation was quite sensitive to AMAD (g) and XFIX-N (g), which were used to describe ammonium adsorption and desorption in groundwater layer. On the other hand, the Ox-N load generation was most sensitive to NUPTGT (total annual target for plant uptake of nitrogen). For the OP load generation, XFIX-P (u) describing phosphorus adsorption and desorption in upper layer was relatively more important.

In addition, flow generation related parameters (for example, AGWRC, UZSN and INFILT) were found to have significant impact on the nutrient loadings. An accurate flow simulation is important for further model application. It was also found that most sensitive inputs and parameters became a little more significant in summer, probably associated with intense storm events and higher ET.

Given the shallow and quick-moving nature of streams, nutrient reaction parameters describing chemical and biological processes within streams generally won’t have significant impacts on the nutrient loadings. More attention might need to be given to the pollutant generation processes on lands than the nutrient reactions in streams while calibrating nutrient loadings.

Sensitivity of HSPF model outputs to input parameters in any specific watershed depends on the combined impacts of climate and watershed conditions (Donigian and Love, 2007). Some of the sensitivity results should be able to be applied to other studies with similar conditions. The thorough sensitivity analysis identifying significant processes, inputs and parameters for watershed nutrient simulation is expected to provide useful information for guiding AGCHEM usage.

4.6 References

Bicknell, B.R., Imhoff, J.C., Kittle, J.L., Jobes, T.H., and Donigian, A.S, 2005. Hydrological Simulation Program -Fortran (HSPF). User's manual for release 12.2. U.S.EPA. National Exposure Research Laboratory, Athens, GA.

Borah, D.K., Yagow, G., Saleh, A., Barnes, P.L. , Rosenthal, W., Krug, E.C., and Hauck, L.M., 2006. Sediment and nutrient modeling for TMDL development and implementation. *Transactions of the ASABE,* 49 (4): 967-986.

Donigian, A. S., Bicknell, B. R., Patwardham, A. S., Linker, L. C., and Chang, C., 1994. Chesapeake Bay Program: watershed model application to calculate bay nutrient loadings. U.S. EPA-903-R-94-042, Chesapeake Bay Program Office. U.S.EPA. Annapolis, Maryland.

Donigian, A. S., Imhoff, J.C., and Kittle, J.L., 1999. HSPFParm, An Interactive Database of HSPF Model Parameters. Version 1.0. EPA-823-R-99-004. Prepared for U. S. EPA, Office of Science and Technology, Washington, D. C.

Donigian, A.S., and Love, J.T., 2007. The Housatonic River Watershed Model: Model Application and Sensitivity/Uncertainty Analysis. 7th International IWA Symposium on System Analysis and Integrated Assessment in Water Management, May 7-9, 2007. Washington, DC.

Fontaine, T. A., and Jacomino, V. M. F, 1997. Sensitivity analysis of simulated contaminated sediment transport. JAWRA 33: 313-326.

Hantzche, N. N., and Finnemore, E.J., 1991. Predicting ground-water nitrate-nitrogen impacts. Groundwater, 30 (4): 490-499.

Im, S., Brannan, K.M., and Mostaghimi, S., 2003. Simulating Hydrology and Water Quality Impacts in an Urbanizing Watershed. JAWRA 39(6): 1465-1479.

Kieffer, J.M., 2002. Development of a nutrient and dissolved oxygen water quality model for the Saint Louis Bay watershed. M.S. thesis. Mississippi State University.

Liu, Z., Kieffer, J. M., Hashim, N.B., Kingery, W.L., and Huddleston, D.H., 2005. The Influence of Crop Fertilization Practices on Nutrient Input Parameters for Water Quality Modeling in the Wolf River Watershed Using HSPF. International Journal of Civil and Environmental Engineering. 1(1): 1-17.

Liu, Z., Kingery, W.L., Huddleston, D. H., Hossain, F., Hashim N. B., and Kieffer J. M., 2008. Application and evaluation of two nutrient algorithms of Hydrological Simulation Program Fortran in Wolf River watershed. Journal of Environmental Science and Health, Part A 43(7):738-48.

Liu, Y., Godrej, A.N., and Grizzard, T.J., 2011a. Sensitivity Analysis, Calibration and Validation of a Watershed Model Application using HSPF with the Nutrient Algorithm PQUAL in Upper Broad Run Watershed, VA. In Submission.

Marshall, J., 2009. Personal Communication. Fauquier County Soil and Water Conservation District, Virginia.

Neitsch, S.L., Arnold, J.R., Kiniry, J.R., Williams, J.R. and King, W.K. 2002. Soil and Water Assessment Tool Theoretical Documentation Version 2000. Texas Water Resources Institute, College Station, Texas.

Ohlwiler, T., 2009. Personal Communication. Fauquier County Cooperative Extension Office, Virginia.

Saleh, A, and Du, B., 2004. Evaluation of SWAT and HSPF within BASINS Program for the Upper North Bosque River Watershed in Central Texas, Transactions of the ASAE. 47(4): 1039-1049.

Shoemaker, L., Dai, T., Koenig, J., and Hantush, M., 2005. TMDL model evaluation and research needs. EPA/600/R-05/149.Cincinnati, Ohio: U.S. EPA, National Risk Management Research Laboratory.

United States Department of Agriculture (USDA), 1992. Agricultural Waste Management Field Handbook. Natural Resources Conservation Service, Washington, DC

United States Environmental Protection Agency (USEPA), 2002. National Water Quality Inventory 2000 Report. EPA-841-R-02-001, Washington, DC.

U.S. Department of Agriculture (USDA), 2004. National Agricultural Statistics Service. 2002 census of agriculture. Available at http://www.nass.usda.gov/census.
Virginia Department of Conservation and Recreation (VDCR), 2005. Virginia Nutrient Management Standards and Criteria.

Wu, J., 2004. Water-quality-based BMP design approach and uncertainty analysis for integrated watershed management. PhD. Dissertation, University of Virginia.

White, K. L. and Chaubey, I., 2005. Sensitivity Analysis, Calibration, and Validations for a Multisite and Multivariable SWAT Model. Journal of American Water Resources Association 41(5):1077-1089.

Young, R.A., Onstad, C.A., Bosch, D.D. and Anderson, W.P. 1994. Agricultural Non-Point Source Pollution Model, Version 4.03 AGNPS User's Guide, U.S. Department of Agriculture, Washington, D.C.

Chapter 5. Comparison of Two Nutrient Simulation Algorithms of HSPF in Upper Broad Run Watershed, Virginia

Yingmei Liu[1], Adil N. Godrej[2], and Thomas J. Grizzard[3]
[1]*PhD graduate, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*
[2]*Research Associate Professor, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*
[3]*Professor, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*

5.1 Abstract

This study conducted a side by side comparison of two nutrient simulation algorithms of HSPF: PQUAL and AGCHEM. The comparison was based on HSPF applications, using either PQUAL or AGCHEM in the Upper Broad Run watershed, a 126.21 km^2 rural watershed in Fauquier County, Virginia. Both applications were calibrated for a four-year simulation period (2002-2005) and validated for a two-year simulation period (2006-2007). The model performances for simulated nutrient loadings from the watershed and in-stream nutrient concentrations were compared.

Both PQUAL and AGCHEM provided good to reasonable predictions of nutrient loads and concentrations during the calibration and validation periods. Simulated nutrient concentrations were similar. AGCHEM performed slightly better than PQUAL for predicting OP (orthophosphate phosphorus) concentrations during the validation period. Nutrient load comparison results show more differences between the two algorithms. Overall, AGCHEM performed better than PQUAL for predicting OP loads. For NH_4-N (ammonium nitrogen) and Ox-N (oxidized nitrogen), although both algorithms did equally well in simulating the annual loads, PQUAL provided a better fit between simulated and observed seasonal and monthly loads. This was possibly associated with the quality of nitrogen fertilizer input data used for the AGCHEM application.

5.2 Introduction

Nitrogen and phosphorus are essential nutrients for plants and aquatic organisms. However, excessive amounts in waterbodies can trigger eutrophication with undesired algal growth, hypoxia, high turbidity, and fish death (Wetzel, 2001). These problems will eventually impair recreation, aesthetics, and other beneficial uses of the waterbodies. To address this issue, TMDLs (total maximum daily load) is required under the Clean Water Act for each impaired waterbody included in the State 303 (d) List. As defined by USEPA (1999), a TMDL is "a calculation of the maximum amount of a pollutant that a waterbody can receive and still meet water quality standards and an allocation of that amount to the pollutant's sources".

Computational models have been used to simulate watershed hydrology and water quality processes. Some of the watershed models are often used to support development of nutrient TMDLs, typically to identify nutrient sources and characterize timing of the nutrient loadings from a watershed. The Hydrological Simulation Program-FORTRAN (HSPF) is one of the most-used watershed models for nutrient assessment and comprehensive TMDL studies (Borah et al., 2006). Since being included in the USEPA Better Assessment Science Integrating Point and Nonpoint Sources (BASINS) package, HSPF has been widely applied in various geographic regions for watershed nutrient simulation (for example, Rahman and Salbe, 1995; Bergman et al., 2002; Cerco et al., 2002; Im et al., 2003; Liu et al., 2008).

HSPF allows for algorithms that vary in complexity for nutrient simulation on pervious and imperious lands and within streams in a watershed. To estimate nutrient losses on pervious land areas, the primary choice is between using the simpler empirical method PQUAL or the more complex process-oriented method AGCHEM. PQUAL assumes simple relationships of nutrient losses with water and sediment yield. AGCHEM applies a nutrient balance approach as the foundation for simulating complex nutrient transport and reactions in the soil explicitly. Both PQUAL applications (for example, Bergman et al., 2002; El-Kaddah and Carey, 2004; Xu, 2005) and AGCHEM applications (for example, Donigian et al., 1994; Im et al., 2003; Saleh and Du, 2004) have been found for watershed nutrient simulation.

For a particular HSPF application, selection between the simple empirical algorithm PQUAL and the complex physical-based algorithm AGCHEM is a challenging task. Generally, modelers tend to select PQUAL due to its ease of use. AGCHEM is more difficult to apply because of extensive data requirement, complicated module setup, and lack of modeling guidance (Liu et al., 2008). On the other hand, AGCHEM may provide a better nutrient simulation as a physical-based method. Nasr et al. (2007) compared three physical-based models (HSPF with AGCHEM, SWAT and SHETRAN/GOPC) and two empirical models (DM and ECM) for modeling phosphorus export from three catchments in Ireland. Compared to the simple empirical models, the three physically-based models gave annual TP export estimates closer to the measurements. In contrast, other studies comparing models that shared many common features but differed in model complexity found that more mechanistic models didn’t greatly improve model predictions (for example, Gao et al., 2004 and Skinner et al., 2008).

However, a review of the literature shows that little has been published on comparative analyses of PQUAL and AGCHEM. Liu et al (2008) replaced PQUAL with AGCHEM to simulate nutrient losses from pasture and crop lands in the Wolf River watershed. It was found that the inclusion of AGCHEM module didn’t significantly improve model performance in simulating in-stream nutrient concentrations. Possibly this was because AGCHEM was only applied in a small percentage (12.4%) of the total area and thus made little to no difference to the simulation results. The study didn’t indicate the difference between simulated nutrient loadings from the watershed by replacing PQUAL with AGCHEM. For nutrient TMDL development, accurate estimation of magnitude and timing of nutrient loadings from the watershed is very important.

The principal objective of the research reported here was to conduct a side by side comparison of the nutrient simulation algorithms of HSPF: PQUAL and AGCHEM. The study was conducted based on an HSPF application, one using PQUAL and one using AGCHEM, in the Upper Broad Run basin, a 126.21 km^2 rural watershed in Fauquier County, Virginia. Both applications were calibrated for a four-year simulation period (2002-2005) and validated for a two-year simulation period (2006-2007). The model performances in simulating nutrient loadings from the watershed and in-stream nutrient concentrations were compared. In addition, this study provided an overview of important inputs and parameters describing PQUAL and AGCHEM, and their indications for simulating nutrient management practices. It is hoped that findings from this study would help modelers in making an informed decision regarding HSPF algorithm selection for watershed nutrient assessment, nutrient TMDL development and implementation.

5.3 Materials and Methods

5.3.1 Study Area

The Upper Broad Run watershed is a 126.21 km^2 basin that lies in Fauquier County and drains to Lake Manassas, Virginia. The basin is located in the upper part of the larger Occoquan watershed in the Northern Virginia suburbs of Washington, DC (Figure 5-1). The climate in the study area is humid-subtropical with four distinctive seasons. The average annual air temperature and precipitation are about 13.2 ℃ and 101.6 cm, respectively.

The stream station ST70 at the outlet of the watershed (Figure 5-1) has been monitored by the Occoquan Watershed Monitoring Laboratory (OWML) for both flow and water quality since 1978. Flow is monitored once per hour for baseflow conditions, and every 15 minutes during storm events. For baseflow conditions, water quality grab samples are taken on a weekly basis, except for biweekly during the winter season. Composite flow-weighted storm water quality samples are collected automatically during storm events.

Figure 5-1 also shows the rain gages in the Occoquan watershed. Precipitation data from AIRL (Airlie), RITC (C. Hunter Ritchie Elementary School), and CSNY (Camp Snyder wetlands) were used for this study. Other meteorological data were obtained from Washington Dulles International Airport weather station (DULL). These data included air temperature, cloud cover, dew point temperature, potential evapotranspiration (ET), solar radiation, wind speed and precipitation.

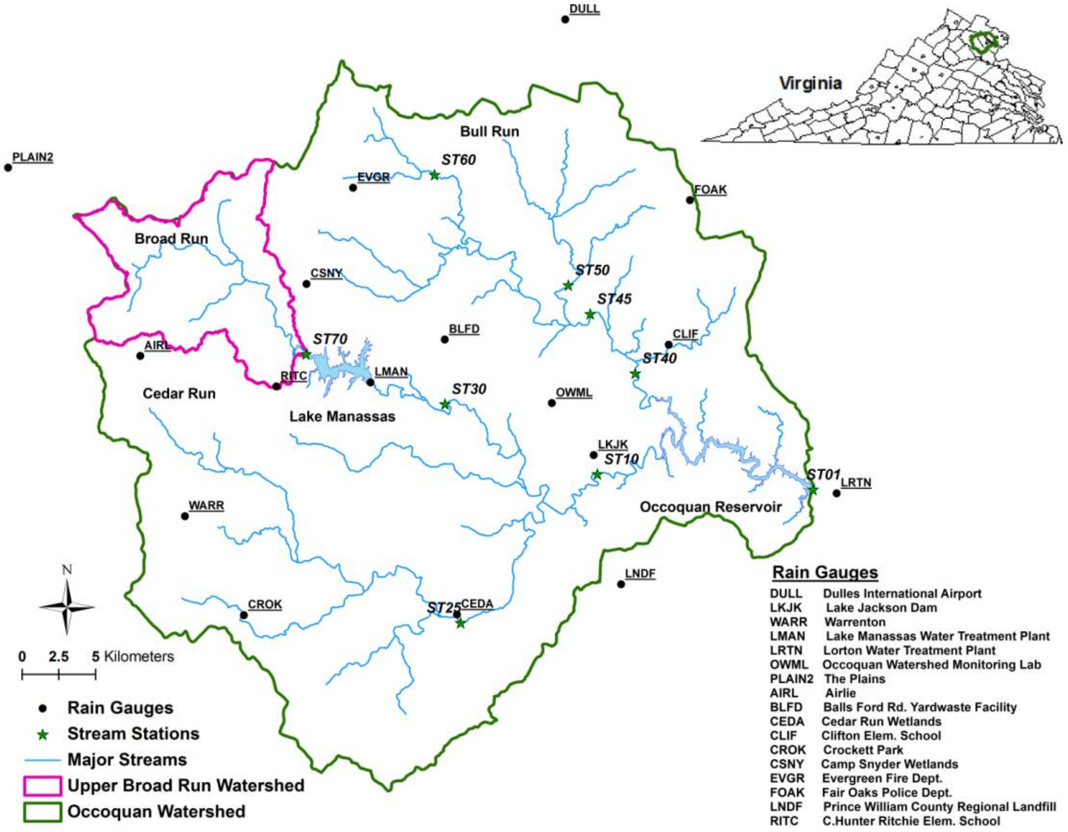


Figure 5-1: Location of Upper Broad Run Watershed, Showing Major Streams, Stream Stations and Rain Gauges in the Occoquan Watershed

Most of the study area falls into the Foothills subprovince in the Piedmont Region physiographic province, characterized by moderate slopes and relatively high elevations from 400 ft (121.92 m) to 1000 ft (304.8 m). The soils are generally loam and moderately well-drained. Based on the 2006 land use data from the Northern Virginia Regional Commission (NVRC), the majority of the study area is rural. The land use distribution is

63.3% of forest, 20.9% of pasture, 9.9% of cropland, and 5.9% of urban. The major grass is cool season turf grass including tall fescue grass and Kentucky blue grass. The main crops are hay, corn, wheat and soybean.

5.3.2 Model Description

HSPF simulates nutrient processes in three modules—PERLND, IMPLND, and RCHRES. The PERLND module includes two algorithms for nutrient simulation on pervious lands: a simpler empirical method PQUAL, or a more detailed physical method AGCHEM. The IMPLND module uses IQUAL (similar to PQUAL) to simulate nutrient export from impervious lands. There is no counterpart for AGCHEM in the IMPLND module, as AGCHEM processes describe only those occurring on pervious areas. After the nutrient fluxes from the pervious and impervious lands are transported to streams, several physical and biochemical processes are simulated under the RCHRES module. Detailed descriptions of these modules can be found in Bicknell et al. (2005) and Donigian et al. (1995).

Two HSPF applications using PQUAL and AGCHEM for nutrient simulation on pervious lands were developed in the Upper Broad Run watershed (Liu et al., 2011a; Liu et al., 2011b). Both applications were developed using 7 segments in the simulation period from 2002 to 2007 (Figure 5-2).

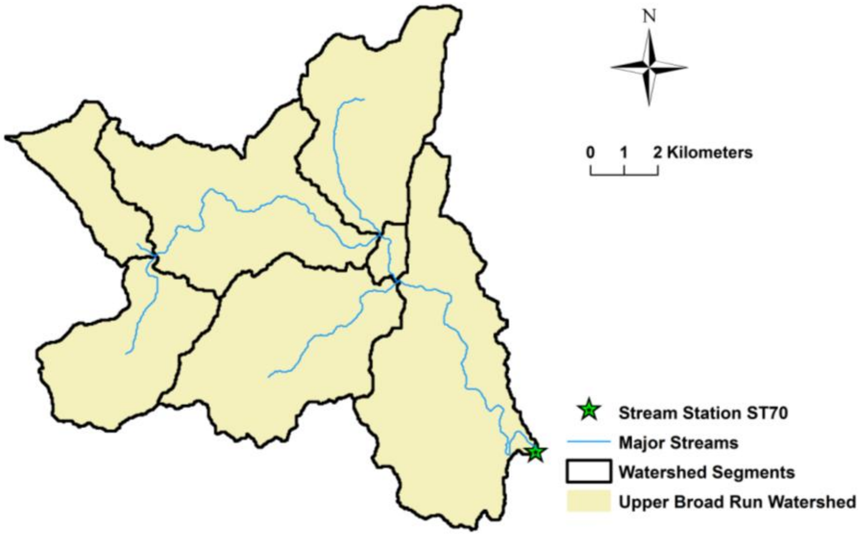


Figure 5-2: Segmentation of the Upper Broad Run Watershed

PQUAL application

Three nutrient species including orthophosphate phosphorus (OP), ammonium nitrogen (NH_4-N) and oxidized nitrogen (Ox-N) were simulated in the PQUAL application. Table 5-1 lists a handful of main PQUAL parameters for simulating NH_4-N, Ox-N and OP separately.

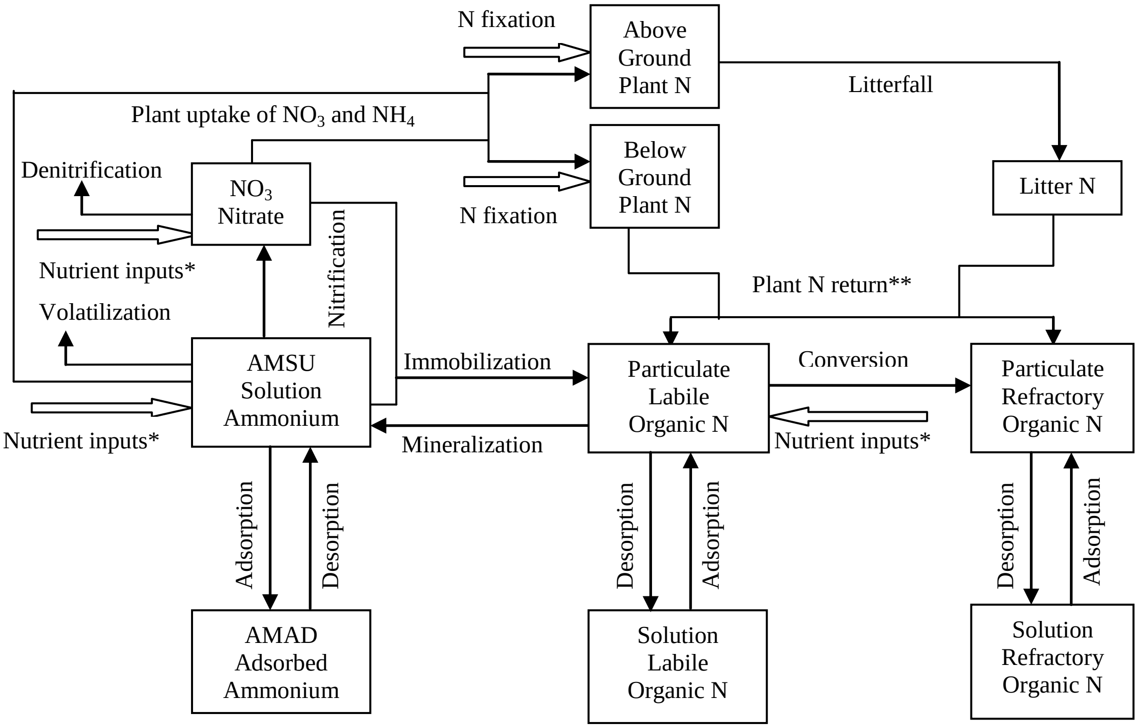
Table 5-1: List of Main PQUAL Parameters for Nitrogen and Phosphorus Simulation

Parameter	Description
	NH_4-N/Ox-N/OP simulation
POTFW-NH_4/NO_3/OP	Washoff potency factor for nutrient (NH_4, NO_3, or OP)
ACQOP-NH_4/NO_3/OP	Accumulation rate of nutrient (NH_4, NO_3, or OP) on the surface
SQOLIM-NH_4/NO_3/OP	Maximum storage of nutrient (NH_4, NO_3, or OP) on the surface
WSQOP-NH_4/NO_3/OP	Rate of surface runoff that will remove 90% of stored nutrient (NH_4, NO_3, or OP) per hour
IFLW-CON-NH_4/NO_3/OP	Interflow nutrient (NH_4, NO_3, or OP) concentration
GRND-CON-NH_4/NO_3/OP	Groundwater nutrient (NH_4, NO_3, or OP) concentration

For each of the nutrient species, PQUAL simulates nutrient fluxes from land surface, interflow and groundwater by assuming simple relationships of nutrient with water and sediment yield. POTFW (washoff potency factor) is used to relate the nutrient yield to sediment removal from land surface. The nutrient yield from land surface is also estimated based on a function of storage quantity and overland flow, called “buildup and washoff”. ACQOP (accumulation rate) and SQOLIM (maximum storage capacity) are used to simulate nutrient buildup during dry periods. WSQOP (rate of surface runoff that will remove 90% of stored nutrient per hour) is used to relate nutrient washoff to surface runoff during wet periods. The nutrient fluxes in interflow and active groundwater are estimated by multiplying flow and user-defined concentrations (IFLW-CON and GRND-CON).

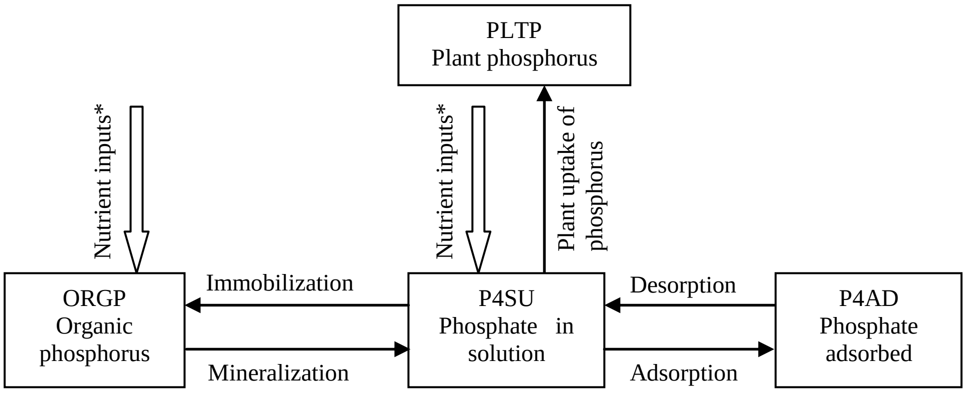
AGCHEM application

The AGCHEM algorithm applies a nutrient balance approach as the foundation for simulating complex nutrient processes in the soil explicitly, including nutrient inputs from atmospheric deposition, fertilization and manure application, and subsequent nutrient movement and transformation as well as plant uptake in the soil profile. The soil profile is divided into four layers for moisture and nutrient storage, including surface, upper, lower and groundwater. AGCHEM includes NITR (Figure 5-3) and PHOS (Figure 5-4) sections for nitrogen and phosphorus simulation, respectively.



* Nutrient inputs from atmospheric deposition, fertilization and manure application
**Return of above ground plant N and litter N occurs to surface and upper layers only

Figure 5-3: Flow Diagram for Nitrogen Reactions by NITR (redrawn from Bicknell et al., 2005)



* Nutrient inputs from atmospheric deposition, fertilization and manure application

Figure 5-4: Flow Diagram for Phosphorus Reactions by PHOS (redrawn from Bicknell et al., 2005)

Details about the development of the AGCHEM application in the Upper Broad Run watershed were described in another paper (Liu et al., 2011b). The general information for important components of the nutrient balance is briefly described below.

Nutrient reactions

The general nutrient processes simulated in the AGCHEM application included adsorption and desorption, mineralization and immobilization, nitrification and denitrification, and plant uptake. Tables 5-2 and 5-3 list the main AGCHEM parameters used for simulating the general nitrogen and phosphorus processes in four soil layers.

Table 5-2: List of Main AGCHEM Parameters Used for Nitrogen Simulation

Method	Parameter	Description
Adsorption and desorption of NH_4		
Freundlich isotherm method	XFIX-N (s, u, l, g)*	Maximum ammonium concentration permanently fixed to the soil
	K1-N (s, u, l, g)*	Coefficient for ammonium Freundlich adsorption and desorption equation
	N1-N (s, u, l, g)*	Exponent for ammonium Freundlich adsorption and desorption equation
	AMAD (s, u, l, g)*	Initial storage of adsorbed ammonium
	AMSU (s, u, l, g)*	Initial storage of solution ammonium
Mineralization of organic nitrogen and immobilization of NH_4 & NO_3		
First-order kinetics method	KAM (s, u, l, g)*	Organic nitrogen ammonification rate
	THKAM	Temperature correction factor for organic nitrogen ammonification
	KIMAM (s, u, l, g)*	Ammonium immobilization rate
	THKIMA	Temperature correction factor for ammonium immobilization
	KIMNI (s, u, l, g)*	Nitrate immobilization rate
	THKIMN	Temperature correction factor for nitrate immobilization
Nitrification and denitrification		
First-order kinetics method	KNI (s, u, l, g)*	Nitrification rate
	THKNI	Temperature correction factor for nitrification
	KDNI (s, u, l, g)*	Denitrification rate
	THKDNI	Temperature correction factor for denitrification
Plant uptake of NH_4 & NO_3		
Yield-based method (crop lands)	NH4UTF (NO3UTF)	Fraction of nitrogen uptake from ammonium (nitrate)
	NUPTGT	Total annual target for plant uptake of nitrogen
	NUPT-FR1	Monthly fraction of the annual nitrogen uptake target
	NUPT-FR2 (s, u, l, g)*	Soil layer fraction of the monthly nitrogen uptake
Saturation kinetics method (forest)	CSUAM (s, u, l, g)*	Ammonia half saturation constant for plant uptake
	NITUPAM (s, u, l, g)*	Maximum plant uptake rate for ammonia
	CSUNI (s, u, l, g)*	Nitrate half saturation constant for plant uptake
	NITUPNI (s, u, l, g)*	Maximum plant uptake rate for nitrate
First-order kinetics method (other lands)	NITUPT (s, u, l, g)*	Plant nitrogen uptake rate
	THPLN	Temperature correction factor for plant nitrogen uptake

*Different parameters for 4 soil layers (s: surface layer; u: upper layer; l: lower layer; g: groundwater layer)

Table 5-3: List of Main AGCHEM Parameters Used for Phosphorus Simulation

Method	Parameter	Description
		Adsorption and desorption of PO_4
Freundlich isotherm method	XFIX-P (s, u, l, g)*	Maximum phosphorus concentration permanently fixed to the soil
	K1-P (s, u, l, g)*	Coefficient for phosphorus Freundlich adsorption and desorption equation
	N1-P (s, u, l, g)*	Exponent for phosphorus Freundlich adsorption and desorption equation
	P4AD (s, u, l, g)*	Initial storage of adsorbed phosphate
	P4SU (s, u, l, g)*	Initial storage of solution phosphate
		Mineralization of organic phosphorus and immobilization of PO_4
First-order kinetics	KMP (s, u, l, g)*	Organic phosphorus mineralization rate
	THKMP	Temperature correction factor for organic phosphorus mineralization
	KIMP (s, u, l, g)*	Phosphate immobilization rate
	THKIMP	Temperature correction factor for phosphate immobilization
		Plant uptake of PO_4
Yield-based method (crop lands)	PUPTGT	Total annual target for plant uptake of phosphorus
	PUPT-FR1	Monthly fraction of the annual phosphorus uptake target
	PUPT-FR2 (s, u, l, g)*	Soil layer fraction of the monthly phosphorus uptake
First-order kinetics method (other lands)	PHOSUPT (s, u, l, g)*	Plant phosphorus uptake rate
	THPLP	Temperature correction factor for plant phosphorus uptake

*Different parameters for 4 soil layers (s: surface layer; u: upper layer; l: lower layer; g: groundwater layer)

Fertilizer and manure inputs

The modeled land use types under fertilization included pasture, hay, corn (high tillage corn and low tillage corn), wheat and soybean. Fertilizer was also applied for mixed cool season tall fescue grass and Kentucky blue grass grown in pervious urban areas, including industrial, institutional, low density residential (LDR), medium density residential (MDR) and townhouse. Generally, one typical fertilizer application (including application rate, timing and technique) was developed separately for each fertilized land use, based on recommendations from the Virginia Nutrient Management Standards and Criteria (VDCR, 2005) and personal discussions with Fauquier county extension agents (Marshall, 2009; Ohlwiler, 2009). The typical fertilizer application was applied to all model segments throughout the watershed and assumed to repeat every year over the entire simulation period. Manure was only applied for pasture, with an application rate calculated by dividing the amount of animal waste produced from beef by the acres of pasture (Liu et al., 2011b).

For modeling purposes, the estimated nutrient inputs from fertilizer and manure were included as monthly fluxes into soil in the forms of NH_4, NO_3, organic nitrogen, PO_4, and organic phosphorus. As shown in Figures 5-5 and 5-6, most nitrogen and phosphorus inputs were in spring from March to May.

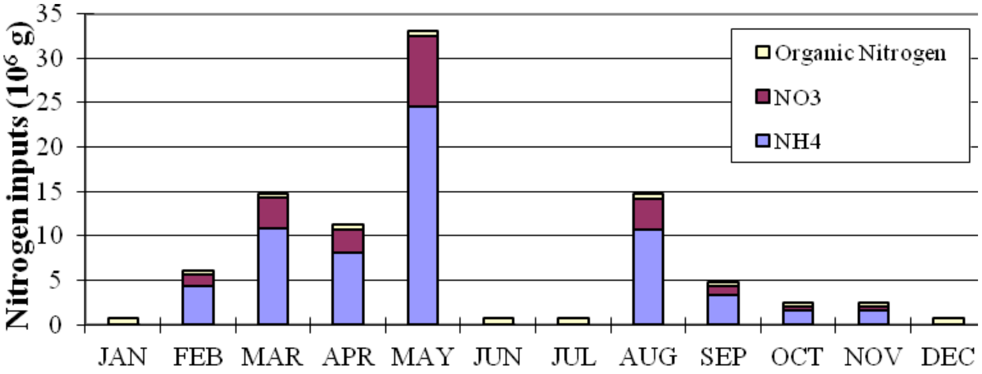


Figure 5-5: Nitrogen Inputs from Fertilizer and Manure

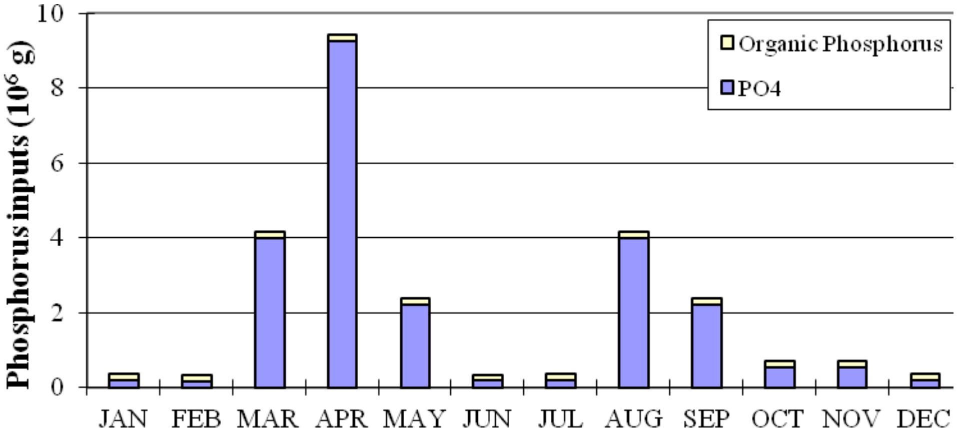


Figure 5-6: Phosphorus Inputs from Fertilizer and Manure

Fertilizer application was very important for the nutrient load generation simulated by AGCHEM (Liu et al., 2011b). The nutrient loads were positively correlated with the fertilizer application rate. Changing fertilizer application time showed significant impacts on seasonal nutrient loads. Therefore, uncertainties associated with the fertilizer application could impact nutrient load generation significantly. On the other hand, the sensitivity of AGCHEM to fertilizer application rate and timing indicates its potency of evaluating the alternative nutrient management practice.

Use of AGCHEM can track the various components of nutrient balances, such as fertilizer and manure inputs, plant uptakes and nutrient exports. AGCHEM also has the advantage of explicitly simulating the nutrient cycles and interactions between nutrient species in the soil. For example, NH_4 can be converted to NO_3 by nitrification. PQUAL simulates each of the nutrient species independently and assumes no interactions between the nutrient species. However, AGCHEM setup is very complicated and requires many more model inputs and parameters. This can be very time consuming.

5.3.3 Model Performance Evaluation

The observed nutrient (OP, NH_4, Ox-N) data from stream station ST70 were used to compare with the simulated results from the HSPF applications. The agreement between simulated and observed data was evaluated by visual and statistical comparisons during both the calibration (2002-2005) and validation (2006-2007) periods. The statistical comparisons performed were percentage difference (PD), standard coefficient of determination (R^2), and standard deviation (SD). PD, the percentage difference between simulated and observed data was defined as

$$PD = \frac{100 \cdot (Y - X)}{X} \%$$

Where *X* is the observed value, and *Y* is the simulated value.

5.4 Results and Discussion

As discussed by Liu et al. (2011a), the calibration year 2003 had an annual precipitation of 135.9 cm, and was considered as a wet year based on a long-term average precipitation of 101.6 cm from 1951 to 2007. Three other calibration years 2002, 2004 and 2005 were considered to be near-average years, with annual precipitation of 97.0 cm, 106.1 cm and 100.9 cm respectively. The validation period had a near-average year 2006 and a dry year 2007, with annual precipitation of 94.2 cm and 73.4 cm respectively.

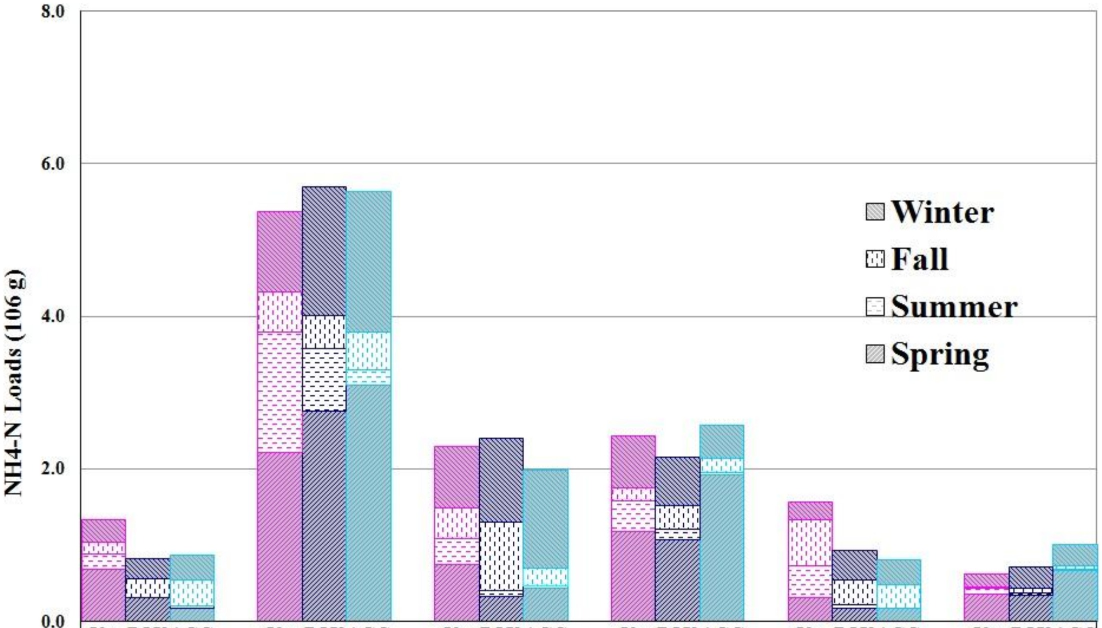
5.4.1 Nutrient Load Comparison Results

The nutrient loads simulated by PQUAL and AGCHEM were compared with observed values on annual, seasonal and monthly scales. Figures 5-7, 5-8 and 5-11 show the nutrient (NH_4-N, Ox-N and OP) comparison results by season for each year during the calibration (2002-2005) and validation (2006-2007) periods. The nutrient loads varied substantially by years and between seasons. Generally, much higher nutrient loads were observed in the wet year 2003. In addition, the nutrient loads were found to be somewhat higher for spring in most years. The statistical comparison results for the annual and seasonal nutrient loads are shown in Tables 5-4 and 5-5. In addition, Figures 5-9, 5-10, 5-12, and Table 5-6 show the comparison results for the monthly nutrient (NH_4-N, Ox-N and OP) loads.

Nitrogen calibration and validation

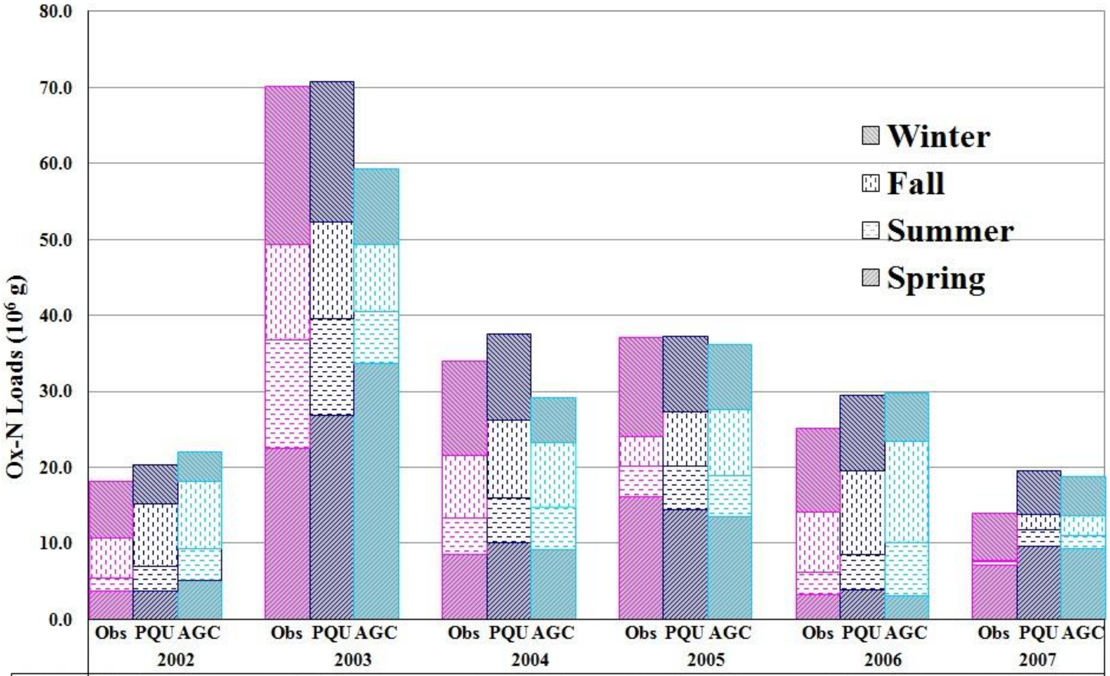
PQUAL and AGCHEM performed equally well for simulating the annual NH_4-N and Ox-N loads. Over the four-year calibration period (2002-2005), the total NH_4-N and Ox-N loads simulated by PQUAL (PD=–3.1% for NH_4-N and PD=+4.1% for Ox-N, Table 5-4) and AGCHEM (PD=–3.2% for NH_4-N and PD=–8.0% for Ox-N, Table 5-4) were very close to the observed values. For both PQUAL and AGCHEM, the PD values of the annual NH_4-N and Ox-N loads were within ±15% for most years during the calibration period (Table 5-4). Over the two-year validation period (2006-2007), there was also no significant difference between the two algorithms for predicting the annual NH_4-N and Ox-N loads.

The comparison results from Figures 5-7, 5-8 and Table 5-5 indicate that AGCHEM generally predicted somewhat higher NH_4-N and Ox-N loads than PQUAL in spring. The largest over-prediction of NH_4-N and Ox-N loads by AGCHEM occurred in March 2003 and May 2003 respectively (Figures 5-9 and 5-10). Since large amounts of Ox-N and NH_4-N from fertilizer are applied in spring, it is expected that AGCHEM will influence the loads more in that season. Compared to AGCHEM, seasonal average NH_4-N loads and Ox-N loads simulated by PQUAL were generally closer to observed values, indicated by relatively lower absolute PD values in Table 5-5. For monthly NH_4-N and Ox-N loads, somewhat higher R^2 values were also found for PQUAL (Table 5-6). These all seemed to indicate that PQUAL captured temporal variations in NH_4-N and Ox-N loads better than AGCHEM.



	2002			2003			2004			2005			2006			2007		
	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC
Total	1.34	0.82	0.87	5.38	5.71	5.64	2.29	2.40	1.99	2.43	2.15	2.57	1.58	0.94	0.80	0.62	0.71	1.01
Winter	0.30	0.27	0.33	1.06	1.69	1.84	0.80	1.10	1.30	0.67	0.63	0.43	0.23	0.39	0.32	0.16	0.28	0.28
Fall	0.16	0.25	0.33	0.52	0.43	0.51	0.42	0.90	0.22	0.17	0.32	0.18	0.60	0.34	0.30	0.02	0.06	0.05
Summer	0.19	0.01	0.03	1.58	0.82	0.19	0.33	0.08	0.04	0.41	0.14	0.03	0.43	0.04	0.01	0.09	0.03	0.02
Spring	0.69	0.31	0.18	2.22	2.77	3.11	0.75	0.32	0.43	1.18	1.07	1.92	0.31	0.17	0.17	0.36	0.35	0.66

Figure 5-7: Comparison of Annual and Seasonal NH_4-N Loads, 2002-2007. (Obs: observed; PQU: PQUAL simulated; AGC: AGCHEM simulated)



	2002			2003			2004			2005			2006			2007		
	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC
Total	18.2	20.4	22.1	70.2	70.8	59.3	34.0	37.6	29.2	37.1	37.3	36.2	25.2	29.5	29.8	13.9	19.6	18.8
Winter	7.48	5.13	3.96	20.8	18.5	9.91	12.3	11.3	5.84	12.9	9.94	8.48	11.0	9.92	6.33	6.19	5.71	5.18
Fall	5.28	8.33	8.84	12.6	12.6	8.91	8.35	10.1	8.60	3.97	7.19	8.66	7.94	11.0	13.4	0.13	2.13	2.55
Summer	1.62	3.16	4.19	14.1	12.8	6.80	4.69	5.88	5.58	3.95	5.71	5.44	2.94	4.74	6.91	0.54	2.13	1.76
Spring	3.85	3.83	5.16	22.5	26.9	33.7	8.65	10.1	9.23	16.2	14.5	13.6	3.30	3.86	3.19	7.12	9.66	9.35

Figure 5-8: Comparison of Annual and Seasonal Ox-N Loads, 2002-2007. (Obs: observed; PQU: PQUAL simulated; AGC: AGCHEM simulated)

Table 5-4: Comparison of Annual Percent Differences (PD) of Nutrient (NH_4-N, Ox-N, OP) Loads, 2002-2007

		Calibration					Validation		
		2002	2003	2004	2005	Total (2002-2005)	2006	2007	Total (2006-2007)
NH_4-N	PQUAL	–38.4%	+6.1%	+4.8%	–11.4%	–3.1%	–40.6%	+15.2%	–24.9%
	AGCHEM	–34.8%	+4.9%	–13.1%	+5.8%	–3.2%	–49.1%	+63.5%	–17.5%
Ox-N	PQUAL	+12.2%	+0.9%	+10.5%	+0.6%	+4.1%	+17.1%	+40.3%	+25.4%
	AGCHEM	+21.5%	–15.6%	–14.1%	–2.5%	–8.0%	+18.4%	+34.8%	+24.2%
OP	PQUAL	+3.8%	–4.7%	+14.9%	–28.7%	–5.9%	–65.2%	–56.2%	–61.7%
	AGCHEM	–20.5%	–25.9%	+7.3%	+8.3%	–11.2%	–33.5%	–13.6%	–25.7%

Table 5-5: Comparison of Seasonal Average Percent Differences (PD) of Nutrient (NH_4-N, Ox-N, OP) Loads for Calibration (2002-2005) and Validation (2006-2007) Periods

		Spring (March – May)		Summer (June – August)		Fall (September – November)		Winter (December –February)	
		PQUAL	AGCHEM	PQUAL	AGCHEM	PQUAL	AGCHEM	PQUAL	AGCHEM
NH_4-N	Calibration	–7.7%	+16.5%	–58.5%	–88.3%	+49.8%	–2.1%	+30.5%	+38.3%
	Validation	–22.4%	+25.3%	–86.5%	–94.3%	–35.0%	–43.1%	+68.3%	+52.6%
Ox-N	Calibration	+8.0%	+20.2%	+12.7%	–9.9%	+26.6%	+15.7%	–16.1%	–47.5%
	Validation	+29.7%	+20.3%	+97.1%	+149.1%	+63.3%	+98.2%	–9.4%	–33.3%
OP	Calibration	+0.1%	+14.6%	–28.1%	–46.2%	–16.7%	–11.6%	+15.5%	–16.8%
	Validation	–66.7%	–9.4%	–53.8%	–7.1%	–72.2%	–42.4%	–33.5%	–24.0%

Table 5-6: Comparison of Monthly R^2 of Nutrient (NH_4-N, Ox-N, OP) Loads for Calibration (2002-2005) and Validation (2006-2007) Periods

	NH_4-N		Ox-N		OP	
	PQUAL	AGCHEM	PQUAL	AGCHEM	PQUAL	AGCHEM
Calibration	0.474	0.270	0.741	0.407	0.604	0.818
Validation	0.275	0.177	0.657	0.305	0.352	0.430

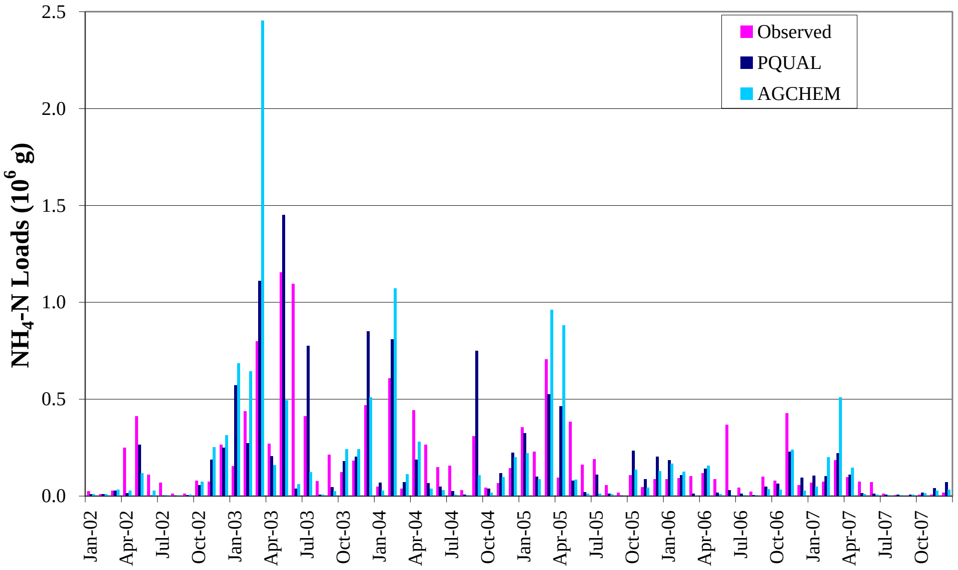


Figure 5-9: Comparison of Monthly NH_4-N Loads, 2002-2007

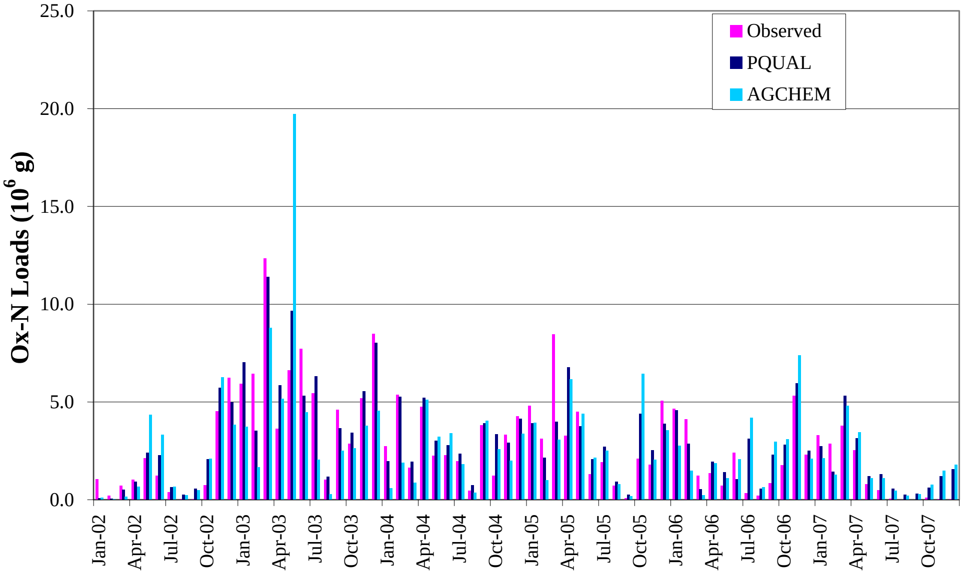
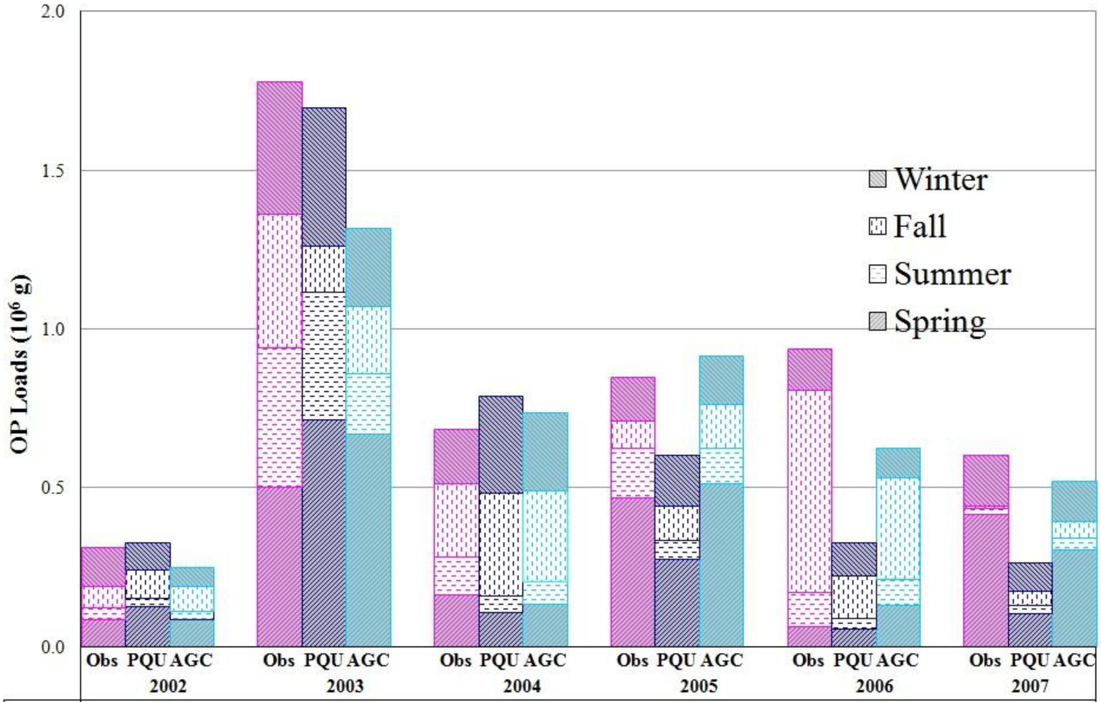


Figure 5-10: Comparison of Monthly Ox-N Loads, 2002-2007

Phosphorus calibration and validation

There are relatively more differences between the OP loads simulated by PQUAL and AGCHEM. During the calibration period, the large differences occurred in 2003 (PD=–4.7% for PQUAL and PD=–25.9% for AGCHEM, Table 5-4) and 2005 (PD=–28.7% for PQUAL and PD=+8.3% for AGCHEM, Table 5-4). The low absolute PD values of seasonal average OP loads in Table 5-5 and high R^2 values of monthly OP loads (0.604 for PQUAL and 0.818 for AGCHEM, Table 5-6) indicate that both algorithms were able to capture temporal variations in OP loads well. Based on a close investigation of the monthly OP loads (Figure 5-12), AGCHEM performed slightly better for predicting higher OP loads (such as May 2003, July 2003 and March 2005).

Both PQUAL and AGCHEM generally underestimated the OP loads in the validation years of 2006 and 2007. However, the magnitudes underestimated by AGCHEM (PD=–33.5% for 2006 and PD=–13.6% for 2007, Table 5-4) were much less than those by PQUAL (PD=–65.2% for 2006 and PD=–56.2% for 2007, Table 5-4). For PQUAL, the large differences were mainly due to under-prediction of higher OP loads in November 2006 and March 2007 (Figure 5-12), which might help explain the large PD values in predicting the fall (PD=–72.2%, Table 5-5) and spring (PD=–66.7%, Table 5-5) average OP loads.



	2002			2003			2004			2005			2006			2007		
	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC	Obs	PQU	AGC
Total	0.31	0.33	0.25	1.78	1.70	1.32	0.69	0.79	0.74	0.85	0.60	0.92	0.94	0.33	0.62	0.60	0.27	0.52
Winter	0.13	0.08	0.06	0.42	0.43	0.25	0.17	0.30	0.25	0.14	0.16	0.15	0.13	0.10	0.09	0.16	0.09	0.13
Fall	0.07	0.09	0.08	0.42	0.15	0.21	0.23	0.33	0.28	0.09	0.11	0.14	0.64	0.14	0.32	0.01	0.04	0.05
Summer	0.04	0.03	0.03	0.44	0.40	0.19	0.12	0.05	0.07	0.15	0.06	0.11	0.11	0.03	0.08	0.02	0.03	0.04
Spring	0.09	0.13	0.08	0.50	0.71	0.67	0.16	0.11	0.13	0.47	0.27	0.51	0.06	0.05	0.13	0.42	0.10	0.31

Figure 5-11: Comparison of Annual and Seasonal OP Loads, 2002-2007. (Obs: observed; PQU: PQUAL simulated; AGC: AGCHEM simulated)

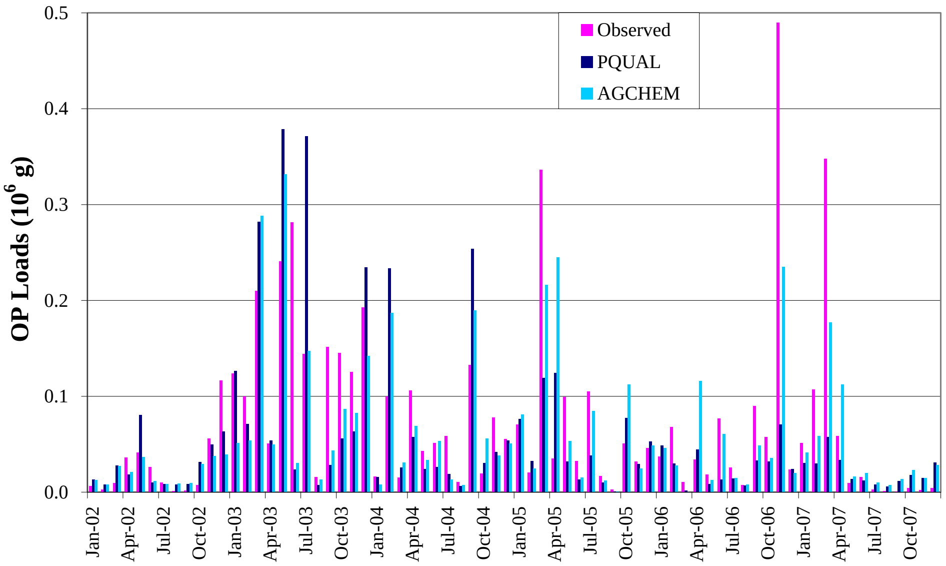


Figure 5-12: Comparison of Monthly OP Loads, 2002-2007

Overall, AGCHEM performed better than PQUAL for predicting OP loads. For NH_4-N and Ox-N, although both algorithms did equally well in simulating the annual loads, PQUAL captured temporal variations in the loads better than AGCHEM. This is likely associated with the quality of input data used for this AGCHEM application. The typical nutrient application assumed for each land use type throughout the watershed during the entire simulation period may not accurately represent site-specific practices. For example, some pasture and hay land areas are not receiving nitrogen fertilizer every year (Marshall, 2009). If data are available, a more complicated nutrient input method “special action block” might overcome the limit. With the special action block, the nutrient input could be changed at a specified time to simulate human activities (Bicknell et al., 2005).

5.4.2 Nutrient Concentration Comparison Results

For each of the nutrients, there were, respectively, 247 and 103 observed sample data for the calibration (2002-2005) and validation (2006-2007) periods. Comparisons of nutrient concentrations are presented as time series plots (Figures 5-13, 5-15, 5-17), and as box-and-whisker plots (Figures 5-14, 5-16, 5-18) separated by season and type of flow (baseflow and storm). Each box graphs the quartiles with the lower and upper edges representing the 25th and 75th percentiles, respectively. The midline is the median value. The open square is the average value. The asterisks are the maximum and minimum values. In addition, Tables 5-7, 5-8 and 5-9 show the statistical comparison results for nutrient (NH_4-N, Ox-N, OP) concentrations. Concentration data below the detection limit was set to one-half the detection limit.

Nitrogen calibration and validation

Both PQUAL and AGCHEM were able to predict the general trends in observed NH_4-N concentrations (Figure 5-13). As shown in Table 5-7 and Figure 5-14, storm NH_4-N concentrations were generally higher and showed greater variation than baseflow concentrations. For both PQUAL and AGCHEM, the absolute differences between average observed and simulated storm NH_4-N concentrations were less than 0.009 mg/l during the calibration and validation periods (Table 5-7). In summer and fall, the peak storm NH_4-N concentrations simulated by PQUAL were somewhat higher than the values simulated by AGCHEM (Figures 5-13 and 5-14). For baseflow NH_4-N concentrations, there was not much difference between PQUAL and AGCHEM, and both algorithms generally underestimated the concentrations especially in summer (Table 5-7 and Figure 5-14).

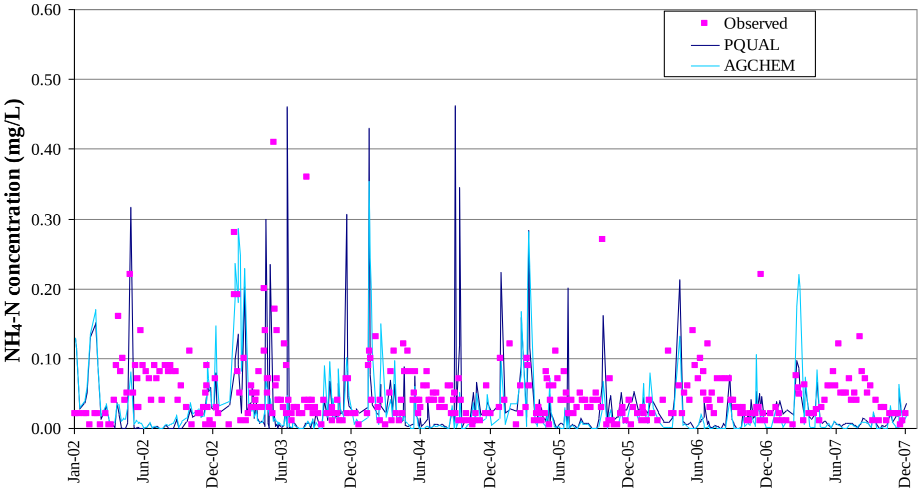


Figure 5-13: Comparison of NH_4-N Concentrations, 2002-2007

Table 5-7: Comparison of NH_4-N Baseflow and Storm Concentrations for Calibration (2002-2005) and Validation (2006-2007) Periods

	Calibration (2002-2005)						Validation (2006-2007)					
	Baseflow			Storm			Baseflow			Storm		
	Mean	SD	Diff*	Mean	SD	Diff*	Mean	SD	Diff*	Mean	SD	Diff*
Observed (mg/l)	0.038	0.032		0.076	0.072		0.038	0.030		0.053	0.044	
PQUAL (mg/l)	0.017	0.025	–0.021	0.080	0.105	+0.004	0.012	0.011	–0.026	0.051	0.042	–0.002
AGCHEM (mg/l)	0.018	0.032	–0.020	0.067	0.077	–0.009	0.008	0.011	–0.030	0.060	0.065	+0.007

* Difference

Table 5-8: Comparison of Ox-N Baseflow and Storm Concentrations for Calibration (2002-2005) and Validation (2006-2007) Periods

	Calibration (2002-2005)						Validation (2006-2007)					
	Baseflow			Storm			Baseflow			Storm		
	Mean	SD	Diff*	Mean	SD	Diff*	Mean	SD	Diff*	Mean	SD	Diff*
Observed (mg/l)	0.561	0.267		0.631	0.170		0.394	0.253		0.491	0.127	
PQUAL (mg/l)	0.728	0.168	+0.167	0.689	0.100	+0.058	0.709	0.163	+0.315	0.658	0.118	+0.167
AGCHEM (mg/l)	0.546	0.262	–0.015	0.671	0.362	+0.040	0.633	0.208	+0.239	0.785	0.249	+0.294

* Difference

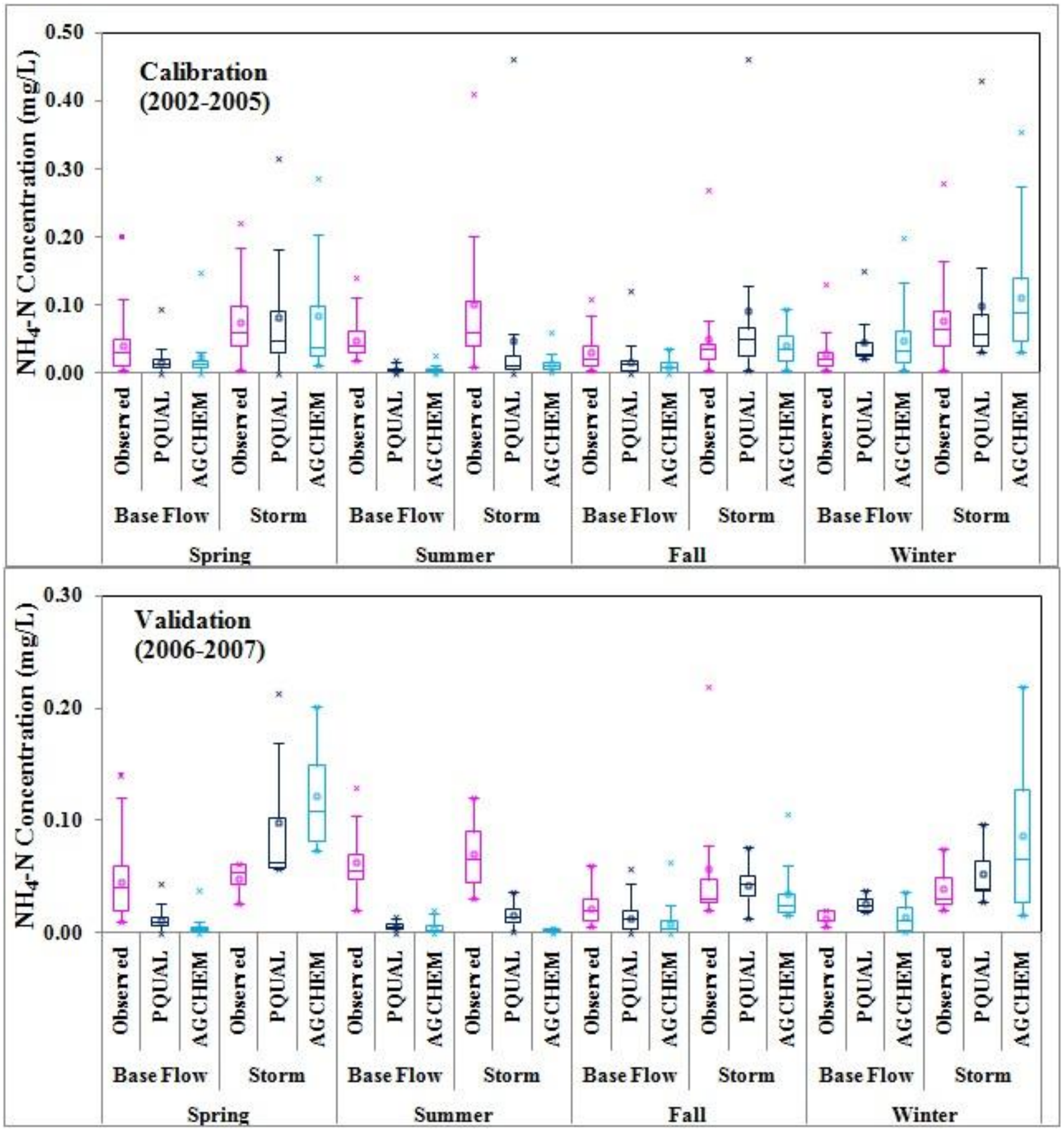


Figure 5-14: Seasonal Comparison of Baseflow and Storm NH_4-N Concentrations for Calibration (2002-2005) and Validation (2006-2007) Periods

Differences between PQUAL and AGCHEM were more apparent for Ox-N concentrations. Although the magnitudes of Ox-N concentrations simulated by both algorithms were in the range of observed data, the Ox-N concentrations simulated by PQUAL didn’t show as large a variation as observed data did (Figures 5-15 and 5-16). This was partially because PQUAL used fairly constant user-defined monthly interflow and groundwater concentration values for Ox-N simulation. During the calibration period, the absolute differences between the average observed and simulated Ox-N concentrations were small for both baseflows (0.015 mg/l for AGCHEM and 0.167 mg/l for PQUAL, Table 5-8) and storm flows (0.040 mg/l for AGCHEM and 0.058 mg/l for PQUAL, Table 5-8). As shown in Table 5-8 and Figure 5-16, both algorithms generally overestimated the baseflow and storm Ox-N concentrations during the validation period.

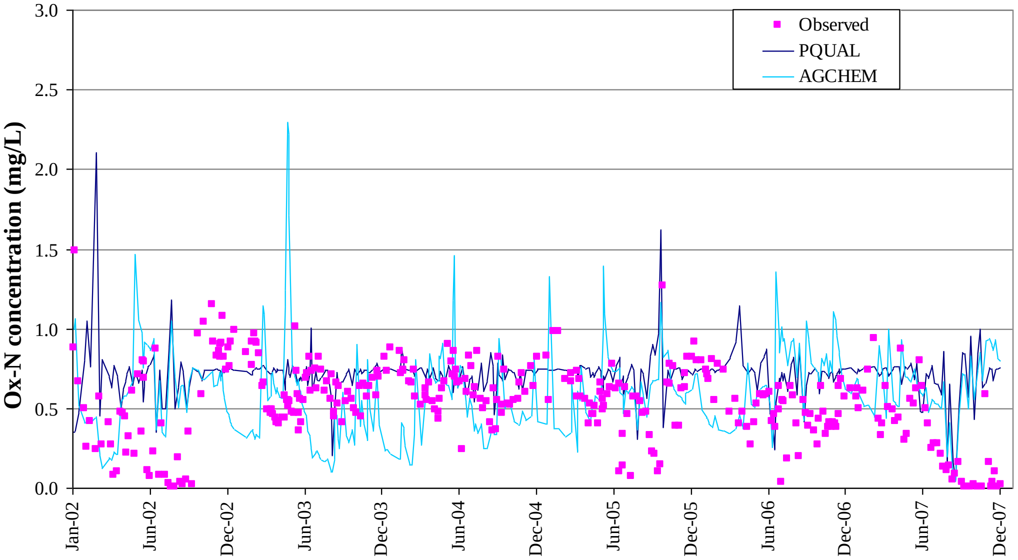


Figure 5-15: Comparison of Ox-N Concentrations, 2002-2007

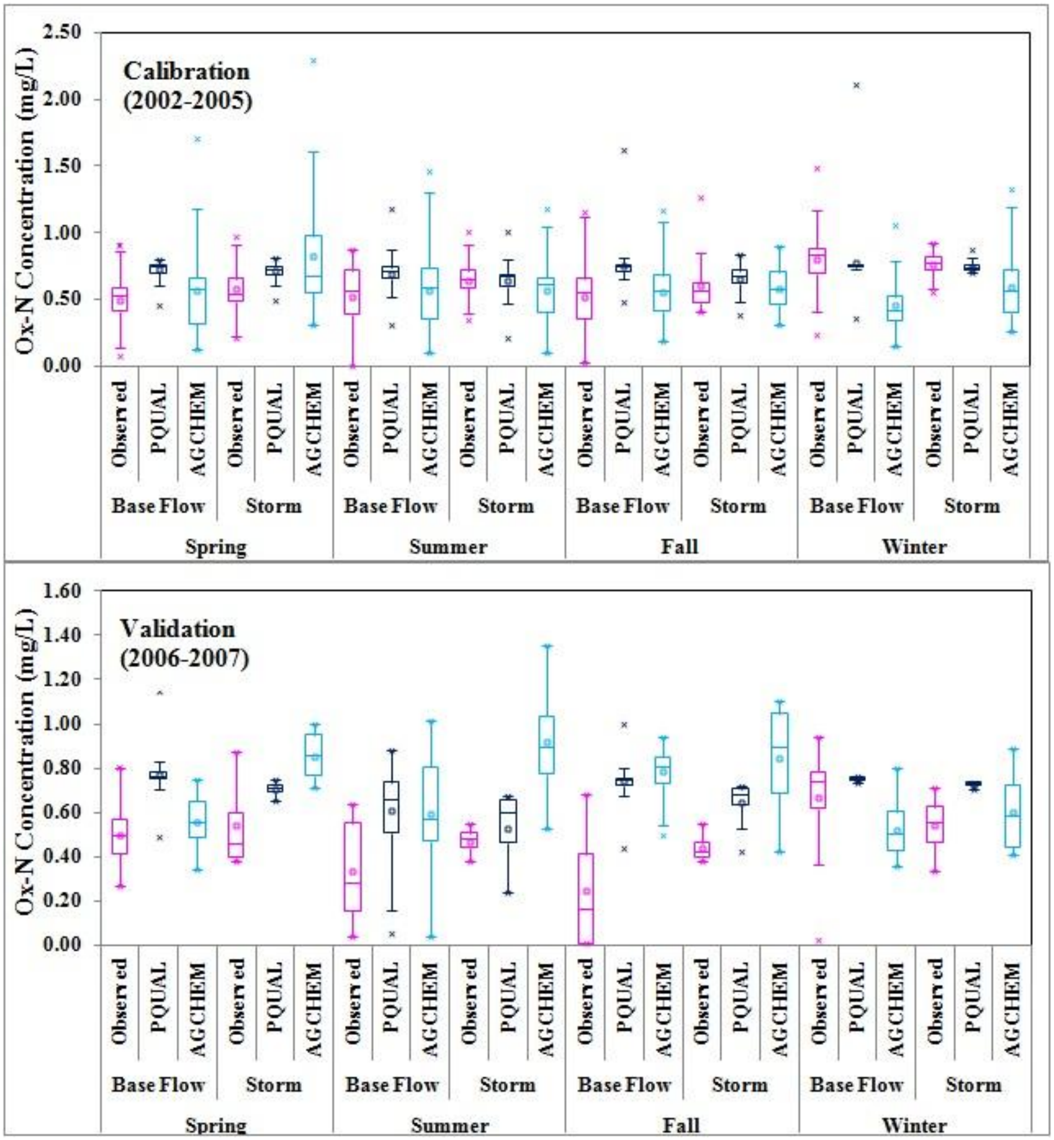


Figure 5-16: Seasonal Comparison of Baseflow and Storm Ox-N Concentrations for Calibration (2002-2005) and Validation (2006-2007) Periods

Phosphorus calibration and validation

The time series plot of OP concentration (Figure 5-17) does not show much difference between PQUAL and AGCHEM. Both algorithms predicted the general trends of observed OP concentrations reasonably well. The high observed OP concentrations during the validation years of 2006 and 2007 were not captured by either of the algorithms.

During the calibration period, the absolute differences between average observed and simulated OP concentrations were small for both baseflows (0.001 mg/l for PQUAL and 0.002 mg/l for AGCHEM, Table 5-9) and storm flows (0.003 mg/l for PQUAL and 0.002 mg/l for AGCHEM, Table 5-9). Both PQUAL and AGCHEM also demonstrated good performance in capturing the seasonal trends for both baseflows and storm flows (Figure 5-18).

During the validation period, observed storm OP concentrations were significantly higher and showed greater variation than baseflow data in all the seasons (Figure 5-18). Although both algorithms didn't reproduce this well, storm OP concentrations simulated by AGCHEM were closer to observed values, especially in spring. As shown in Table 5-9, the absolute difference between the average observed and simulated storm OP concentrations was 0.039 mg/l for AGCHEM, less than the absolute difference of 0.055 mg/l for PQUAL.

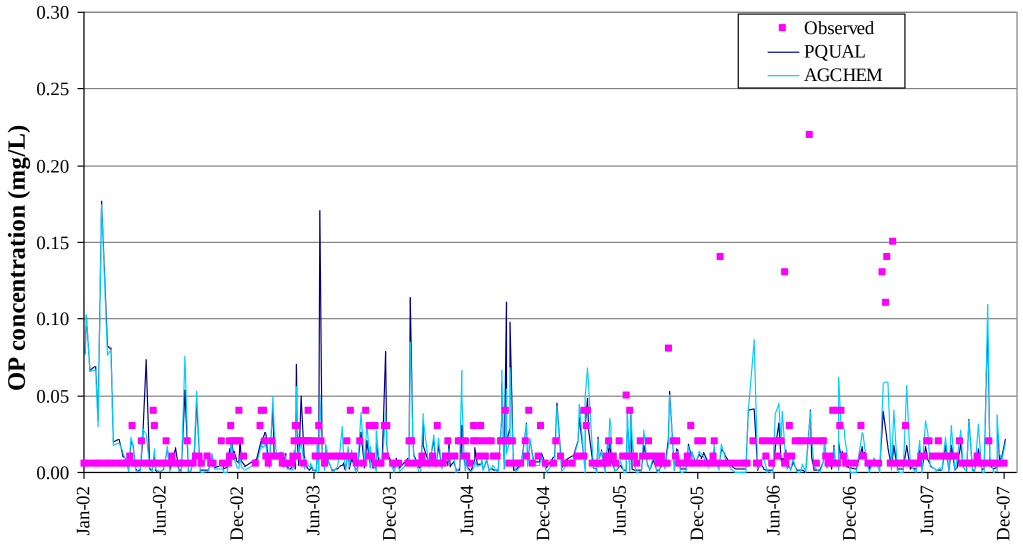


Figure 5-17: Comparison of OP Concentrations, 2002-2007

Table 5-9: Comparison of OP Baseflow and Storm Concentrations for Calibration (2002-2005) and Validation (2006-2007) Periods

	Calibration (2002-2005)						Validation (2006-2007)					
	Baseflow			Storm			Baseflow			Storm		
	Mean	SD	Diff*	Mean	SD	Diff*	Mean	SD	Diff*	Mean	SD	Diff*
Observed (mg/l)	0.009	0.005		0.022	0.013		0.009	0.006		0.072	0.075	
PQUAL (mg/l)	0.010	0.021	+0.001	0.025	0.027	+0.003	0.008	0.013	–0.001	0.017	0.010	–0.055
AGCHEM (mg/l)	0.011	0.022	+0.002	0.024	0.018	+0.002	0.010	0.016	+0.001	0.033	0.021	–0.039

* Difference

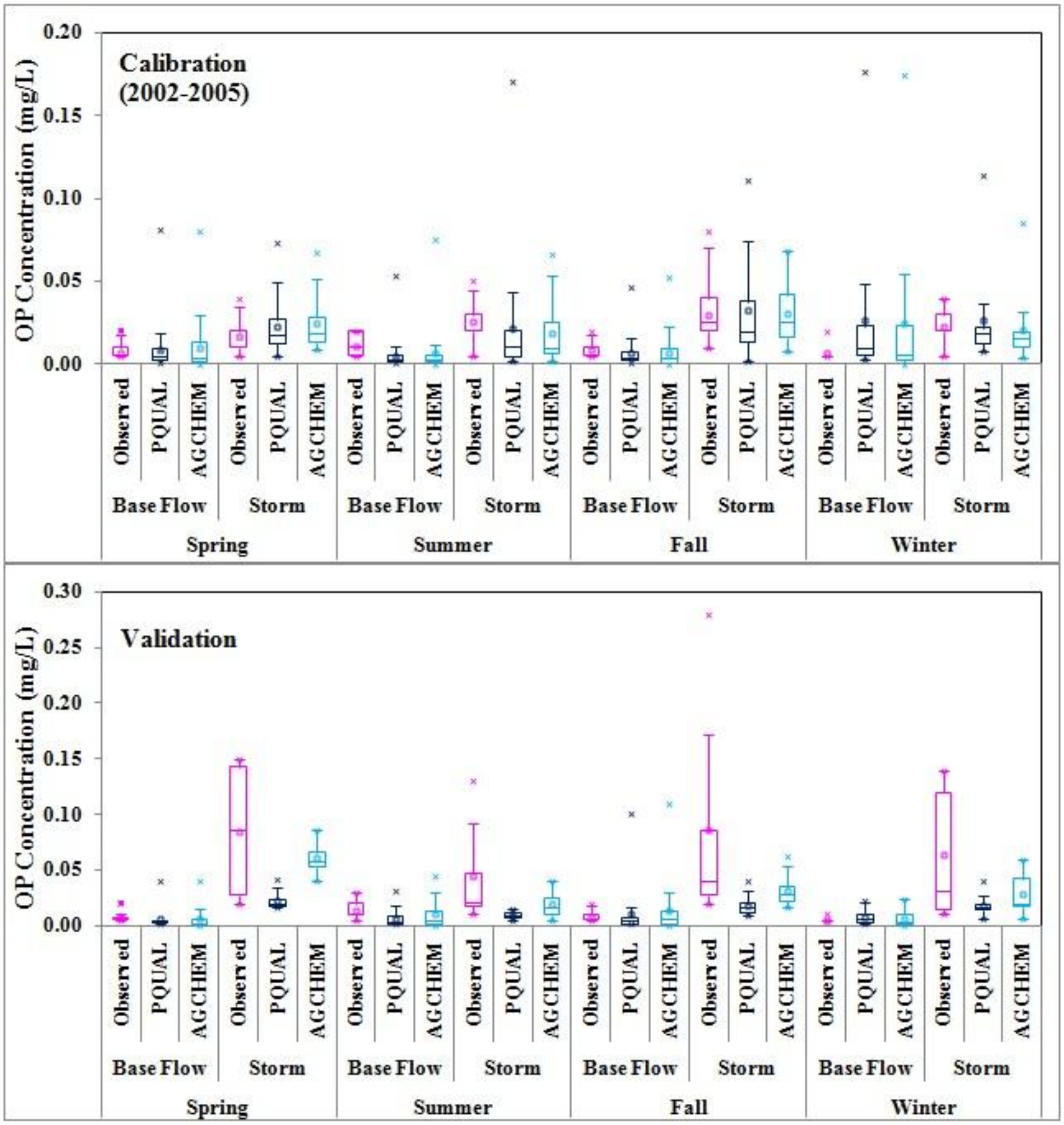


Figure 5-18: Seasonal Comparison of Baseflow and Storm OP Concentrations for Calibration (2002-2005) and Validation (2006-2007) Periods

5.5 Summary and Conclusions

The wide uses of HSPF for watershed nutrient assessment and TMDL studies make it important to evaluate and compare nutrient simulation algorithms PQUAL and AGCHEM. Mechanically, AGCHEM has advantages of explicitly representing the comprehensive nutrient processes and simulating the interactions of nutrient species in the soil. Use of AGCHEM can track nutrient balances such as fertilizer and manure inputs, plant uptakes and nutrient exports. In addition, AGCHEM affords the flexibility to evaluate alternative nutrient management practices. However, compared to PQUAL, AGCHEM is less user-friendly and takes much more time in model development and calibration. A significant concern is if AGCHEM can provide sufficiently more accurate nutrient modeling results than PQUAL, thus making the time and effort involved in using AGCHEM worthwhile.

In the Upper Broad Run watershed, two HSPF applications with PQUAL and AGCHEM were developed and calibrated by using observed data from 2002 to 2005. The two HSPF applications were also validated for a two-year simulation period (2006-2007). The nutrient (OP, NH_4-N, Ox-N) concentration comparison results didn't show much difference between PQUAL and AGCHEM. Both algorithms were able to predict the general trends in observed nutrient concentrations. The simulated Ox-N concentrations by PQUAL didn't show as large a variation from observed data. Compared to PQUAL, storm OP concentrations simulated by AGCHEM were closer to observed values during the validation period.

Both PQUAL and AGCHEM also provided good to reasonable predictions of nutrient loads during the calibration and validation periods. AGCHEM performed better than PQUAL for predicting OP loads. For NH_4-N and Ox-N, although both algorithms did equally well in simulating the annual loads, PQUAL provided a better fit between simulated and observed seasonal and monthly loads. AGCHEM generally predicted somewhat higher NH_4-N and Ox-N loads than PQUAL in spring, when large amounts of nitrogen fertilizer were applied.

Overall, AGCHEM can improve the nutrient modeling performance if accurate inputs and parameters are provided. However, good quality data on the extensive inputs and parameters required by AGCHEM might not be available, which could impact the model performance significantly. For a particular HSPF application, the nutrient algorithm selection needs to consider the data availability, required modeling accuracy, and modelers' time and experience. In addition, the model purpose is another important factor to be considered. As more TMDL studies result in implementation, the use of models for management planning and alternatives analysis is increasing. To investigate management alternatives, models need to provide sensitivity to changes of fertilizer application, tillage, and land cover management (Shoemaker et al., 2005). Compared to PQUAL, AGCHEM has advantage for such complex nutrient TMDL studies.

5.6 References

Bicknell, B.R., Imhoff, J.C., Kittle, J.L., Jobes, T.H., and Donigian, A.S, 2005. Hydrological Simulation Program -Fortran (HSPF). User's manual for release 12.2. U.S.EPA. National Exposure Research Laboratory, Athens, GA.

Bergman, M.J., Green, W., and Donnangelo, L.J., 2002. Calibration of storm loads in the south Prong watershed, Florida, using BASINS/HSPF. Journal of the American water resources association. 38(5): 1423-1236.

Borah, D.K., Yagow, G., Saleh, A., Barnes, P.L., Rosenthal, W., Krug, E.C., and Hauck, L.M., 2006. Sediment and nutrient modeling for TMDL development and implementation. Transactions of the ASABE, 49 (4): 967-986.

Cerco, C.F., Linker, L., Sweeney, J., Shenk, G., and Butt, A.J., 2002. Nutrient and Solid Controls in Virginia's Chesapeake Bay Tributaries. Journal of Water Resources Planning and Management, 128(3): 179-189.

Donigian, A. S., Bicknell, B. R., Patwardham, A. S., Linker, L. C., and Chang, C., 1994. Chesapeake Bay Program: watershed model application to calculate bay nutrient loadings. U.S. EPA-903-R-94-042, Chesapeake Bay Program Office. U.S.EPA. Annapolis, Maryland.

Donigian, A. S., Bicknell, B. R., and Imhoff, J. C., 1995. Hydrologic Simulation Program - FORTRAN. Computer Models of Watershed Hydrology, Water Resources Publications, V. P. Sirgh, ed., Highlands Ranch, CO, 395-442.

El-Kaddah, D.N., and Carey, A.E., 2004. Water quality modeling of the Cahaba River, Alabama. Environmental Geology. 45: 323-338.

Gao, Q., Zhang, X., Huang, Y., and Xu, H., 2004. A comparative analysis of four models of photosynthesis for 11 plant species in the Loess Plateau. Agricultural and Forest Meteorology 126: 203–222.

Im, S., Brannan, K.M., and Mostaghimi, S., 2003. Simulating Hydrology and Water Quality Impacts in an Urbanizing Watershed. JAWRA 39(6): 1465-1479.

Liu, Z., Kingery, W.L., Huddleston, D. H., Hossain, F., Hashim N. B., and Kieffer J. M., 2008. Application and evaluation of two nutrient algorithms of Hydrological Simulation Program Fortran in Wolf River watershed. Journal of Environmental Science and Health, Part A 43(7):738-48.

Liu, Y., Godrej, A.N., and Grizzard, T.J., 2011a. Sensitivity Analysis, Calibration and Validation of a Watershed Model Application using HSPF with the Nutrient Algorithm PQUAL in Upper Broad Run Watershed, Virginia. In Submission.

Liu, Y., Godrej, A.N., Grizzard, T.J., and Dillaha, T. A., 2011b. Application and Sensitivity Analysis of a Watershed Model Application using HSPF with the Nutrient Algorithm AGCHEM in Upper Broad Run Watershed, Virginia. In Submission.

Marshall, J., 2009. Personal Communication. Fauquier County Soil and Water Conservation District, Virginia.

Nasr, A., Bruen, M., Jordan, P., Kiely, G., Moles, R., and Byrne, P., 2007. A comparison of SWAT, HSPF and SHETRAN/GOPC for modeling phosphorus export from three catchments in Ireland. Water Research 41: 1065-1073.

Ohlwiler, T., 2009. Personal Communication. Fauquier County Cooperative Extension Office, Virginia.

Rahman, M., and Salbe, I., 1995. Modeling impacts of diffuse and point source nutrients on the water quality of South Creek catchment. Environment International. 21(5): 597-603.

Saleh, A, and Du, B., 2004. Evaluation of SWAT and HSPF within BASINS Program for the Upper North Bosque River Watershed in Central Texas, Transactions of the ASAE. 47(4): 1039-1049.

Shoemaker, L., Dai, T., Koenig, J., and Hantush, M., 2005. TMDL model evaluation and research needs. EPA/600/R-05/149.Cincinnati, Ohio: U.S. EPA, National Risk Management Research Laboratory.

Skinner, R.H., Corson, M.S., and Rotz, C.A., 2008. Comparison of Two Pasture Growth Models of Differing Complexity. Agricultural Systems 99: 35-43.

United States Environmental Protection Agency (USEPA), 1999. Protocal for developing nutrient TMDLs. EPA 841-B-99-007. Office of Water, Washington, DC.

Virginia Department of Conservation and Recreation (VDCR), 2005. Virginia Nutrient Management Standards and Criteria.

Wetzel, R.G., 2001. Limnology: Lake and River Ecosystems, Third Edition. Academic Press, San Diego, California.

Xu, Z., 2005. A complex, linked watershed-reservoir hydrology and water quality model application for the Occoquan Watershed, Virginia. Ph.D. Dissertation, Virginia Tech.

Chapter 6. Evaluation of Nutrient Management Plans using a Linked Watershed-Reservoir Model

Yingmei Liu[1], Adil N. Godrej[2], Thomas J. Grizzard[3] and John C. Little[4]
[1]*PhD graduate, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*
[2]*Research Associate Professor, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*
[3]*Professor, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*
[4]*Professor, Civil and Environmental Engineering, Virginia Tech, Blacksburg, VA*

6.1 Abstract

The Lake Manassas watershed is a 189 km^2 basin located in northern Virginia that is urbanizing from agricultural uses. Lake Manassas is a major waterbody in the watershed and experiences eutrophication due to nonpoint sources of nutrients from its drainage areas: the Upper Broad Run and Middle Broad Run subbasins. A linked watershed-reservoir model, consisting of two HSPF/AGCHEM models and one CE-QUAL-W2 model, was applied to simulate the hydrology and water quality activities of the lake and the associated drainage areas. The model was calibrated for the years 2002-05, with a validation period of 2006-07. By using the outputs from the calibrated HSPF/AGCHEM models as boundary inputs, the Lake Manassas CE-QUAL-W2 model was adequately calibrated/validated to reproduce water budget, thermal stratification, and algae/nutrient/DO dynamics in the lake.

The calibrated watershed-reservoir model was then used to evaluate water quality benefits of implementing a nutrient management in the watershed. The way the nutrient management plan was evaluated was to take the current simulation and compare it with a pre-BMP scenario. In the current simulation, N and P fertilizer applications were based on the nutrient management plan recommendations of the Virginia Cooperative Extension. The pre-BMP scenario was designed to represent N and P fertilizer application rates 20 years ago, which were estimated to be 110% of the current N fertilizer and 175% of the current P fertilizer. The pre-BMP scenario analysis results

confirmed that without the nutrient management plan, average annual OP (orthophosphate phosphorus) load would have increase by 79.6%, which would have lead to OP enrichment and enhanced algae growth in Lake Manassas.

6.2 Introduction

Among the assessed 42% of total acres of lakes, reservoirs and ponds in the U.S., 45% are considered impaired (USEPA, 2002). The most common pollutants causing impairment are nitrogen and phosphorus. Excessive nitrogen and phosphorus can trigger eutrophication, with resultant accelerated algae growth, increased turbidity and reduced dissolved oxygen (DO). Eutrophic waterbodies are poor drinking water sources and are undesirable for other beneficial water uses.

Nonpoint sources (NPS) of nutrients, resulting from agricultural activities and urban development, have been identified as leading causes of the nutrient impairment (USEPA, 2002). One common approach to control NPS and protect surface waters is by implementing a nutrient management plan, which is defined as the "efficient use of nitrogen and phosphorus to best meet plant needs while also minimizing the impact of these nutrients on water quality" (NRCS, 2006). Both monitoring and modeling methods can be used to characterize NPS and evaluate the nutrient management plan. Of them, modeling is the favored method because it is more effective than monitoring with respect to and because it allows a quick assessment of alternative management scenarios (Bouraoui and Dillaha, 2000).

Watershed models are often used in nutrient management studies. Some examples are the Agricultural Non-Point-Source Pollution Model (AGNPS) (Young et al., 1994), Soil and Water Assessment Tool (SWAT) (Neitsch et al., 2002) and Hydrological Simulation Program–FORTRAN (HSPF) (Bicknell et al., 2005). HSPF is the most extensively used watershed model for long-term continuous simulation in mixed agricultural and urban watersheds (Borah and Bera, 2004). The HSPF model, with its AGCHEM module, provides a detailed simulation of the dynamic and continuous processes that affect the storages and outflow of nutrients from the watershed. HSPF/AGCHEM has been applied in numerous studies for nutrient simulation (e.g., Donigian et al., 1994; Im et al., 2003; Saleh and Du, 2004; Liu et al., 2008).

Many watershed models, like HSPF and SWAT, include simplified reach modules to simulate flow and water quality transport and fate in streams. However, the reach modules assume the streams to be completely mixed and unidirectional, which limits their uses when a watershed drains into larger waterbodies such as lakes and reservoirs. In the larger waterbodies, stratification and mixing mechanisms are of concern, and thus require representation of hydrodynamics and water quality processes in two or three dimensions. As indicated by DePinto et al. (2004), one approach to solve the issue is to link the watershed models to receiving waterbody models, such as the Water Quality Analysis Simulation Program (WASP) (Wool et al., 2003) and CE-QUAL-W2 (Cole and Wells, 2008). The linked model can represent the complex system more accurately and flexibly. In a linked model application, the watershed model estimates water and pollutant loadings into a waterbody, while the receiving water quality model analyzes resulting water quality impacts in the waterbody in response to the loadings.

Several studies have attempted to link watershed and receiving water quality models (e.g. Debele et al., 2006; CBPO, 2004). CE-QUAL-W2 was found to be the most commonly used receiving water quality model in these linked model applications. Flowers et al. (2001) combined SWAT and CE-QUAL-W2 to evaluate the impacts of dairy BMPs and WWTP phosphorus control strategies on lake water quality in the Lake Waco-Bosque River watershed, Texas. Wu (2004) described using HSPF and CE-QUAL-W2 in modeling the Swift Creek watershed in Virginia to help in developing structural urban BMP strategies. Xu (2005) linked six HSPF model applications and two CE-QUAL-W2 model applications for the Occoquan watershed, Virginia. The linked Occoquan model was used to evaluate the impact of land use changes on water quality.

While linkages from the runoff and water quality components of watersheds to waterbodies have been done, applying such linkages for nutrient management study has not been reported in the literature, to the author's knowledge. More specifically, most HSPF applications in the model linkages used PQUAL for nutrient simulation due to insufficient data availability and complications involved with the AGCHEM application. PQUAL is an alternative nutrient algorithm in HSPF, which simulates nutrient generation by assuming a simple relationship with water and sediment yield. Therefore, HSPF/PQUAL does not provide the level of detail and the capabilities needed to simulate nutrient management practices. In addition, it has not been tested if an HSPF/AGCHEM application will work well within a linked watershed-reservoir system to evaluate nutrient management practices.

This paper demonstrates the application of HSPF/AGCHEM within a linked watershed-reservoir model to evaluate a nutrient management plan for the Lake Manassas watershed. The study was conducted based on two HSPF/AGCHEM model applications for the Upper Broad Run and Middle Broad Run subbasins and one CE-QUAL-W2 model application for Lake Manassas. Outputs from the calibrated HSPF/AGCHEM models were used as boundary inputs for the CE-QUAL-W2 model. The objectives of this research were to 1) calibrate and validate the CE-QUAL-W2 model for Lake Manassas; 2) evaluate the impact of the nutrient management plan on nutrient loadings from the Upper Broad Run watershed; and, 3) evaluate the impact of the nutrient management plan on water quality in the Lake Manassas.

6.3 Materials and Methods

6.3.1 Study Area

The Lake Manassas watershed is located in the upper part of the larger Occoquan watershed in the Northern Virginia suburbs of Washington, DC (Figure 6-1). Lake Manassas is a major waterbody in the watershed. The watershed has a total drainage area of about 189 km^2, covering portions of Fauquier County and Prince William County. Broad Run is the principal tributary to Lake Manassas and drains about 129.5 km^2. Several smaller streams scattered around the lake make up the remaining drainage area, and discharge directly into Lake Manassas.

The Lake Manassas watershed is an agricultural (pasture and crops) watershed undergoing urbanization. Based on the 2006 land use distribution provided by NVRC (Northern Virginia Regional Commission), forest has the largest percentage (63.3%), followed by pasture (17.9%), urban (11.3%) and cropland (6.5%). In addition, there are three golf courses located on the north shore of Lake Manassas: Robert Trent Jones International Golf Club, Stonewall Golf Club and the Virginia Oaks Golf Club, covering about 1% of the watershed. The major grass grown in the study area is cool season turf grass including tall fescue grass and Kentucky blue grass. The main crops are hay, corn, wheat and soybean.

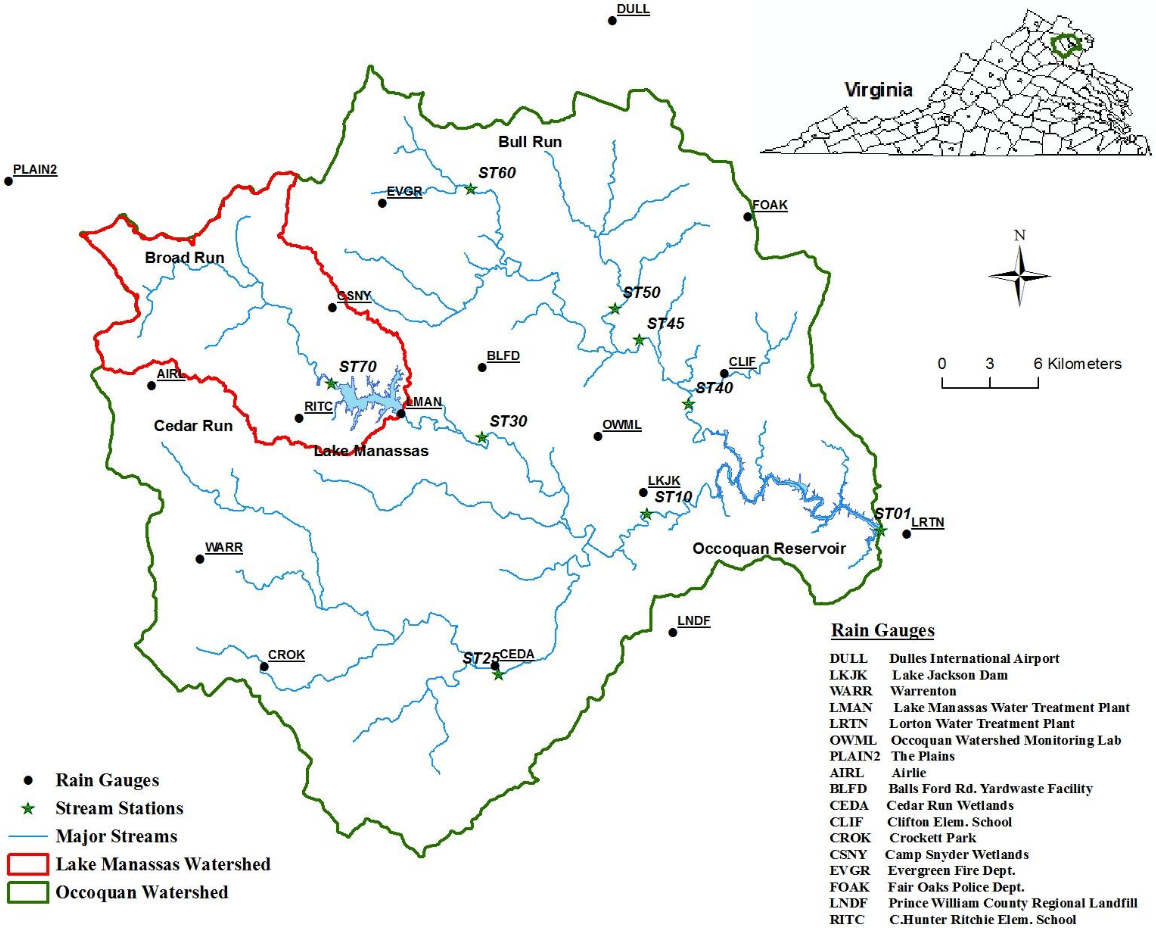


Figure 6-1: Location of Lake Manassas Watershed, Showing Major Streams, Stream Stations and Rain Gauges in the Occoquan Watershed

Lake Manassas was created in the late 1960s by the damming of Broad Run (Gorrie, 2007). Based on a bathymetry survey performed by OWML (Occoquan Watershed Monitoring Laboratory) in 2005, the lake has a storage area of 19.6×10^6 m^3. The lake surface area at the maximum water surface elevation of 88.4 m above mean sea level is 328 hectare. The average depth of the lake is 6.0 m with a maximum depth of approximately 15.0 m near the dam. The lake serves as a drinking water source for the City of Manassas. The City of Manassas Water Treatment Plant withdraws water from three water intakes (primarily the intake at the top) at the dam. The major water quality issue in the lake is eutrophication. Algae growth has consistently created difficulties, including filter clogging along with taste and odor problems, for the water treatment plant operators.

Lake Manassas has been nutrient enriched for a considerable time, and the limiting nutrient is phosphorus (Eggink, 2001). More recently, Gorrie (2007) conducted a limnological investigation of Lake Manassas by using 20 years of monitoring data. Increasing trends of chlorophyll *a* (chl *a*) were observed at all lake stations. The high lake biological productivity was directly related to increasing nutrient levels entering Lake Manassas.

6.3.2 Approach Used to Link the Watershed-Reservoir Model

The Lake Manassas watershed is simulated with two HSPF models (Upper Broad Run and Middle Broad Run) and one CE-QUAL-W2 model (Lake Manassas). As shown in Figure 6-2, the generated flow and pollutant loads from the two HSPF models are fed into CE-QUAL-W2 as boundary inputs for lake hydrodynamic and water quality simulation. The simulation period includes calibration years from 2002 to 2005 and validation years from 2006 to 2007.

Watershed and Lake Segmentation

Figure 6-2 also shows the watershed segmentation. The HSPF models in Upper Broad Run and Middle Broad Run subbasins are developed using 7 and 4 segments, respectively. Some of the segment and reach characteristics are summarized in Table 6-1. Middle Broad Run has relatively short drainage paths and is assumed to drain directly into Lake Manassas.

Table 6-1: Segment and Reach Characteristics of the Upper Broad Run and Middle Broad Run Subbasins

	Upper Broad Run	Middle Broad Run
Number of segments	7	4
Average segment size (km^2)	18.03	15.76
Average elevation (m)	580.71	384.00
Average slope (%)	34.67	17.84
Average reach length (km)	5.43	0.10
Average reach slope (%)	7.53	4.20
Average reach width (m)	6.97	7.40
Average reach depth (m)	0.39	0.40

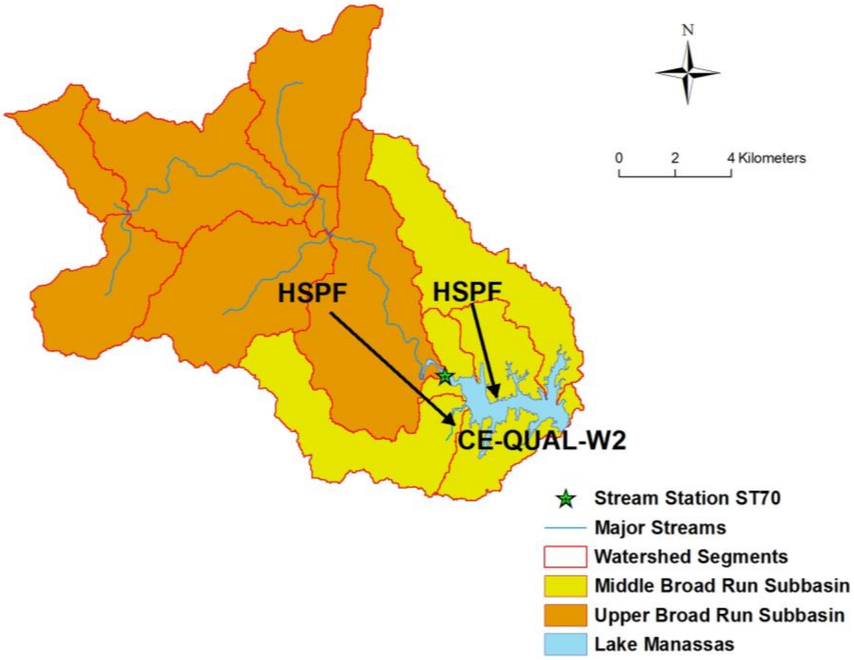


Figure 6-2: Lake Manassas Watershed Model Application Schema and Watershed Segmentation

The lake segmentation used in the CE-QUAL-W2 model is shown in Figure 6-3. Four branches as defined for modeling purposes include the mainstem (branch 1), North Fork (branch 2) and two unnamed arms (branches 3 and 4). The lake is simulated using a total of 32 active computational segments with lengths ranging from 139 m to 691m. Computational layers at full pool range from 1 to 34, each 0.5 m thick.

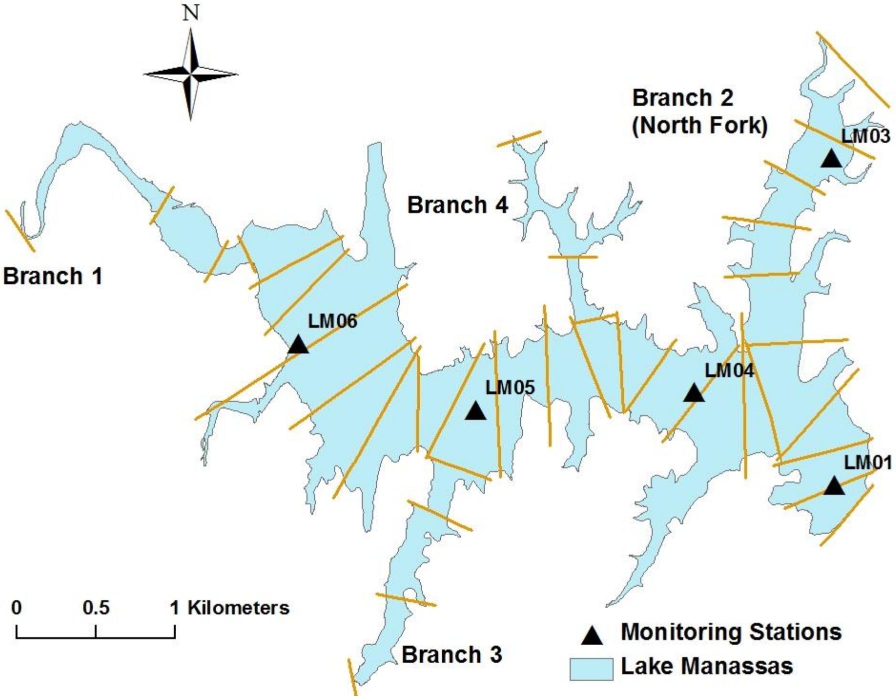


Figure 6-3: Segmentation of Lake Manassas Showing Selected Monitoring Stations

Description of the HSPF Applications

HSPF is a continuous, lumped parameter model designed to simulate various hydrological processes and associated water quality components in a watershed (Bicknell et al., 2005). It is comprised of three application blocks: PERLND, IMPLND, and RCHRES. The PERLND block simulates the hydrological and water quality processes that occur on pervious lands, while IMPLND is used for impervious lands where no infiltration occurs. The RCHRES block simulates the processes that occur in free flow reaches or well-mixed streams. The three application blocks include different routines to simulate runoff, temperature and diverse water quality constituents, including nutrients (nitrogen and phosphorus), carbonaceous biochemical oxygen demand (CBOD), DO, algae and phytoplankton. In this study, nutrient simulation is of primary interest. On the pervious lands, a detailed agricultural chemical approach (AGCHEM) in the PERLND block can be applied to simulate complex nutrient processes in the soil explicitly. These processes include nutrient inputs from fertilization and manure application, as well as subsequent nutrient movements and transformations in four soil layers (surface, upper, lower and groundwater). Nitrogen and phosphorus transformations generally include plant uptake, adsorption and desorption, mineralization and immobilization, nitrification and denitrification. On the impervious lands, nutrient load generation is simulated using IQUAL in the IMPLND block, based on a simple empirical relationship with overland flow and sediment yield. After the nutrient loads are transported from the pervious and impervious lands to the well-mixed streams, several biochemical processes are simulated under the RCHRES block, such as nitrification and denitrification, decay of organic matter, deposition and scour of adsorbed nitrogen and phosphorus.

In the Upper Broad Run subbasin, one HSPF model with the nutrient algorithm AGCHEM was previously developed in the simulation period from 2002 to 2007 (Liu et al., 2011b). This Upper Broad Run model based on HSPF version 12.2 was used here, and detailed procedures about the model development are described elsewhere (Liu et al., 2011a; Liu et al., 2011b). Similar procedures were used to develop the Middle Broad Run HSPF/AGCHEM model in this study. Since Middle Broad Run land areas are assumed to drain directly into Lake Manassas, only PERLND and IMPLND application blocks were used in the Middle Broad Run model.

The HSPF/AGCHEM model requires intensive meteorological data (Table 6-2). In this study, air temperature, cloud cover, dew point temperature, potential evapotranspiration (ET), solar radiation, and wind speed data were obtained from the Washington Dulles International Airport weather station (DULL in Figure 6-1). For the Upper Broad Run model, precipitation data were obtained from AIRL (Airlie), RITC (C. Hunter Ritchie Elem. School), and CSNY (Camp Snyder wetlands). The Middle Broad Run model used precipitation data from RITC, CSNY and LMAN (Lake Manassas Water Treatment Plant). All the meteorological data were input on an hourly time step.

Table 6-2: Meteorological Inputs for the HSPF and CE-QUAL-W2 Models

	HSPF (version 12.2)	CE-QUAL-W2 (version 3.6)
Air Temperature	Required	Required
Cloud Cover	Required	Required
Dew Point Temperature	Required	Required
Potential Evapotranspiration	Required	Not Required
Precipitation	Required	Required
Solar Radiation	Required	Required
Wind Speed	Required	Required
Wind Direction	Not Required	Required

* Based on Xu et al., 2007

The HSPF/AGCHEM model also requires land use and nutrient input data. In this study, 13 land use categories were simulated: forest, golf, pasture, hay, high tillage corn, low tillage corn, wheat, soybean, low density residential, medium density residential, townhouse, institutional, and industrial. The categorization was based on land imperviousness, soil characteristics and several other factors (e.g. planting and harvesting dates, fertilization and manure applications, plant uptakes of nutrients and erosion-related cover). The land use areas were calculated based on 2006 land use data provided by NVRC and county-level cropland distributions of the high tillage and low tillage croplands (Figure 6-4). Cropland distributions in Fauquier and Prince William Counties were estimated based on the 2002 Census of Agriculture from USDA National Agricultural Statistics Service (NASS) (USDA, 2004). Different from the Upper Broad Run model, which used the cropland distribution in Fauquier County, the cropland distribution in Prince William County was used while developing the Middle Broad Run model. The low tillage cropland distributions are similar in the two counties, while the high tillage cropland distributions show a higher percentage of wheat in Prince William County.

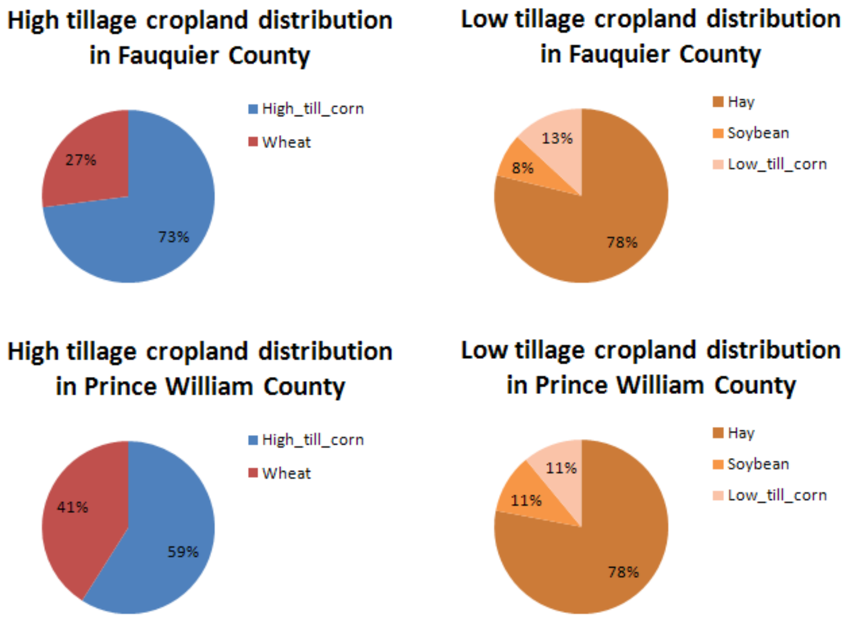


Figure 6-4: High and Low Tillage Cropland Distributions in Fauquier and Prince William Counties

Nutrients from fertilizer, manure, and atmospheric deposition were included as inputs to the HSPF/AGCHEM models. The wet and dry atmospheric deposition of NH_4 (ammonium), NO_3(nitrate) and PO_4 (orthophosphate) were input as monthly fluxes into the surface soil layer for all land use types. Manure was only applied as nutrient input for pasture, and county-level manure deposition rates were estimated based on livestock population density in pasture. For modeling purposes, the developed nutrient inputs from manure were included as monthly fluxes into the surface soil layer in the forms of NH_4, organic nitrogen, PO_4, and organic phosphorus.

Commercial fertilizer was applied as nutrient input for all other land uses except forest. For each fertilized land use type, several steps were taken to develop the fertilizer inputs, including estimating annual fertilizer application rates, distributing the annual rates on a monthly basis, and estimating the distribution of monthly nutrients between the surface and upper soil layers. These were based on recommendations (including application rate, timing and technique) from the Virginia Nutrient Management Standards and Criteria (VDCR, 2005) and personal discussions with Virginia Cooperative Extension and local county extension agents (Ohlwiler, 2009; Marshall, 2009). The developed NH_4, NO_3 and PO_4 inputs from N and P fertilizer for each fertilized land use were included as monthly fluxes into the surface soil and upper soil layers.

Differences between nutrient inputs and data sources used to develop the nutrient inputs for the Upper Broad Run and Middle Broad Run HSPF/AGCHEM models are summarized in Table 6-3. Generally, the manure and fertilizer applications in Fauquier County and Prince William County were used for the Upper Broad Run and Middle Broad Run HSPF/AGCHEM models, respectively. As indicated in Table 6-3, the fertilizer applications were the same for all other land use types except pasture in the two neighboring counties. The differences of manure and fertilizer applications for pasture were mainly because the two counties have different livestock (beef) population densities in pasture.

Table 6-3: Differences between Nutrient Inputs for the Upper Broad Run and Middle Broad Run HSPF/AGCHEM Models

		Upper Broad Run HSPF/AGCHEM model (Fauquier County)	Middle Broad Run HSPF/AGCHEM model (Prince William County)
	Manure application for pasture		
Data sources	Beef population (head)	19206	2321
	Pasture area (ha)	42604	3606
Nutrient inputs	Annual manure NH_4 input (kg/ha/yr)	15.4	22.0
	Annual manure organic N input (kg/ha/yr)	18.9	27.0
	Annual manure PO_4 input (kg/ha/yr)	6.4	9.1
	Annual manure organic P input (kg/ha/yr)	6.4	9.1
	Fertilizer application for pasture		
Data sources	Soil productivity group*	IV	III
	Soil P test level**	32% of the soil P test results are low, 28% medium, 33% high and 7% very high	45% of the soil P test results are low, 38% medium, 13% high and 4% very high
Nutrient inputs	Annual fertilizer PO_4 input (kg/ha/yr)	12.3	16.2

*Based on Virginia Nutrient Management Standards and Criteria (VDCR, 2005) and determined by pasture carrying capacity (acre/animal unit)

**Based on Virginia soil test summary from Virginia Tech Soil Testing Laboratory

Description of the CE-QUAL-W2 Application

CE-QUAL-W2 is a two-dimensional hydrodynamic and water quality model that assumes homogeneity in the lateral direction (Cole and Wells, 2008). It is widely used in relatively long and narrow waterbodies to simulate water surface elevations and describe longitudinal and vertical variations of temperatures and water quality characteristics. CE-QUAL-W2 provides a detailed description of algae/nutrient/DO dynamics and simulates up to 21 water quality constituents, such as CBOD, ammonium, nitrate+nitrite, orthophosphate phosphorus, etc. The simulated nitrogen reactions include respiration and photosynthesis of algae, nitrification, denitrification, anaerobic release from sediment, and decay of organic matter. The processes that affect sinks and sources of phosphorus include growth and respiration of algae, anaerobic release from sediment, decay of organic matter, adsorption, and settling. Oxygen consumption associated with nitrification, decay of organic matter, and respiration and photosynthesis of algae, as well as reaeration are considered in the DO simulation.

CE-QUAL-W2 version 3.6 was used for hydrodynamic and water quality simulation for Lake Manassas. Table 6-2 shows the meteorological data required by the CE-QUAL-W2 model: air temperature, cloud cover, dew point temperature, precipitation, solar radiation, wind speed and wind direction. The Lake Manassas CE-QUAL-W2 model used precipitation data from the LMAN station and other meteorological data from DULL (Figure 6-1). Boundary conditions for the CE-QUAL-W2 model include daily time series of upstream flow, tributary flow, distributed tributary flow, and water withdrawal. Water quality inputs for each of these flows are also required. Upstream flow and associated water quality data were estimated by the Upper Broad Run HSPF/AGCHEM model. The tributary and distributed tributary flows along the lake and associated water quality were estimated by the Middle Broad Run HSPF/AGCHEM model. Water withdrawal data were obtained from the City of Manassas Water Treatment Plant. The CE-QUAL-W2 WaterBalance utility was used to estimate any missing flow, which was then added back into the CE-QUAL-W2 model as distributed tributary flow.

Model Calibration and Validation

The calibration of the linked model was performed in a step-wise manner. First, the Upper Broad Run HSPF model was calibrated using observed data from stream station ST70 (Figure 6-2), which is described in detail elsewhere (Liu et al., 2011a; Liu et al., 2011b). Because the Middle Broad Run subbasin is ungauged, calibration parameters from the Upper Broad Run model were used for the Middle Broad Run model. The outputs from the calibrated Upper Broad Run and Middle Broad Run HSPF models were fed into the Lake Manassas CE-QUAL-W2 model as boundary inputs. The CE-QUAL-W2 model was then calibrated using observed data at five lake stations: LM01, LM03, LM04, LM05 and LM06 (Figure 6-3). The CE-QUAL-W2 calibration started from the water budget calibration and was followed by heat budget calibration and water quality calibration. Water budget calibration was performed by comparing simulated and observed water surface elevation (WSE) at the Lake Manassas dam. Observed WSE data are daily averages collected by OWML. Heat budget calibration was performed by comparing simulated and observed temperature at the five lake stations. Water quality calibration involved DO, OP, NH_4-N (ammonium nitrogen) and Ox-N (oxidized nitrogen) concentration comparisons between simulated and observed values. In each of the lake stations, surface and bottom temperature and other water quality data are collected and analyzed on a biweekly basis during the winter season and on a weekly basis during other seasons. OWML also collects depth profile data for temperature and DO. The profile data are obtained at one-foot, two-and-a-half foot, and five-foot depths, and then at five-foot increments up to the lake bottom. In addition, simulated and observed chl *a* concentration at the lake surface was compared to describe the model’s capability in reproducing algae growth.

Both graphical and statistical methods were applied to evaluate model performance in the calibration and validation periods. Besides the standard coefficient of determination (R^2), several other statistical methods were also used.

Percentage difference (PD) between simulated and observed data was defined as

$$PD = \frac{100 \cdot (Y - X)}{X}\% \qquad (1)$$

Where *X* is the observed value, and *Y* is the simulated value.

In addition, absolute mean error (AME) and root mean square error (RMS) were used to test model performance to reproduce vertical distributions of temperature and DO concentrations. The AMS and RMS between simulated and observed values were defined as

$$AME = \frac{\Sigma\left|\text{Simulated-Observed}\right|}{N} \qquad (2)$$

$$RMS = \sqrt{\frac{\Sigma\left|\text{Simulated-Observed}\right|}{N}} \qquad (3)$$

Where N is number of observations.

6.3.3 Development of Pre-BMP scenario

In this study, the linked model was used to evaluate the water quality benefits of implementing a nutrient management plan. The evaluation was based on a comparison between the current simulation and a pre-BMP scenario. In the current simulation, fertilizer application was based on the recommendations of Virginia Cooperative Extension considering the nutrient management plan. A pre-BMP scenario was designed to represent the fertilizer application 20 years ago.

Based on discussions with a nutrient management specialist at Fauquier County DCR (Marshall, 2009), fertilizer application timing had not changed much in the past 20 years, so that timing did not need to be changed for the pre-BMP scenario. Thus, the pre-BMP scenario only reflected changes in the fertilizer application rate. To simulate the pre-BMP scenario, the fertilizer application rates in the current simulation were multiplied by an application adjustment factor greater than one (1), thus increasing the fertilizer application rate above current conditions. That is, the fertilizer application rate in the pre-BMP scenario was the product of the current fertilizer application rate and an application adjustment factor. The factor was calculated based on fertilizer sales data and land use data in 1985 and 2005. The 1985 and 2005 county-level fertilizer sales data in Virginia were obtained from the Office of Weights and Measures, which tracks product and industry standards in the Virginia Department of Agriculture and Consumer Services. In this study, the calculated application adjustment factor was 1.1 and 1.75 for N and P fertilizer, respectively. They are consistent with findings from the Chesapeake Bay program (Burgholze, 2007): fertilizer application trends have decreased slightly over time for total nitrogen, and have declined significantly for total phosphorus, with an accelerated decline after phytase use began.

In the pre-BMP scenario, watershed segments, waterbody bathymetries, land use data, and all the model input parameters, except the fertilizer application rate, were kept the same as the current scenario. The difference between the model results generated from the two scenarios was used to estimate the water quality benefits of implementing the nutrient management plan. The scenario analysis was conducted at two levels. First, nutrient loads at the outlet of the Upper Broad Run subbasin were compared. The second evaluation was based on water quality (nutrient and chl *a* concentrations) variations at the lake stations.

6.4 Results and Discussion

The model results are presented in two sections. The first section describes the calibration and validation results for the Lake Manassas CE-QUAL-W2 model. The second section describes the pre-BMP scenario analysis results. The model results for the Upper Broad Run HSPF model were described in two other papers (Liu et al., 2011a; Liu et al., 2011b) and won’t be repeated here. In general, the HSPF/AGCHEM model in the Upper Broad

Run subbasin provided a reasonably good prediction of flow and nutrient loadings during the four-year calibration period (2002-2005) and two-year validation period (2006-2007).

6.4.1 Lake Manassas CE-QUAL-W2 Model Calibration and Validation Results

Hydrodynamic Simulation

Figure 6-5 shows an excellent agreement between observed and simulated WSEs at Lake Manassas from 2002 to 2007. The R^2 values were 0.987 and 0.958 in the calibration and validation periods, indicating strong correlations between simulated and observed values.

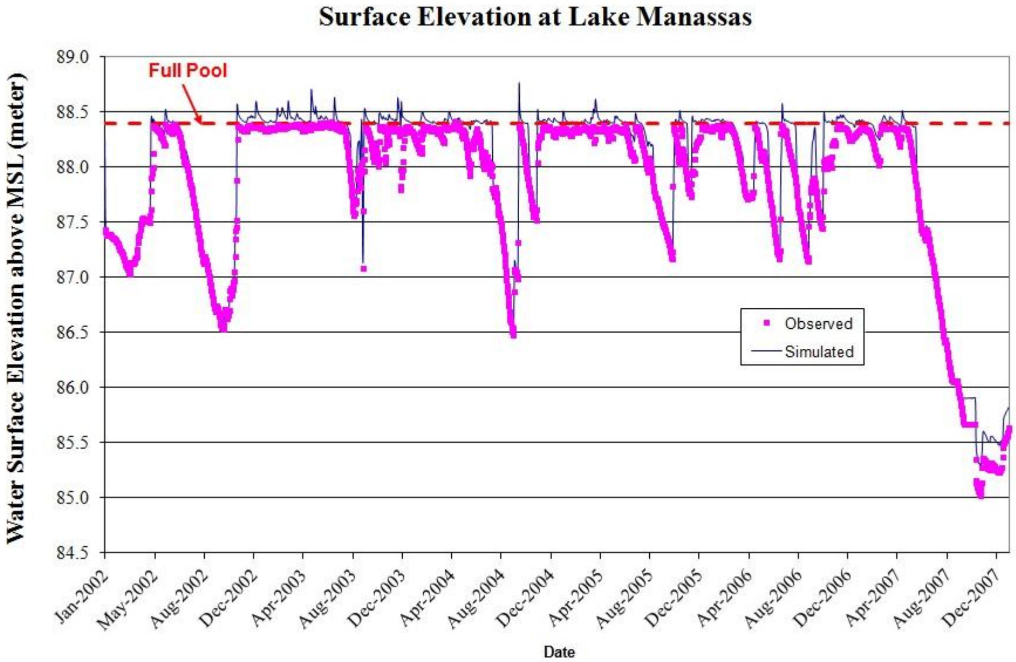


Figure 6-5: Comparison of Water Surface Elevation at Lake Manassas for Model Calibration (2002-2005) and Validation (2006-2007)

Temperature and DO Simulation

The temperature and DO calibration and validation results are presented at LM01, the station near the Lake Manassas dam. The surface condition at this station generally represents the raw water quality going into the City of Manassas Water Treatment Plant, because the plant withdraws water primarily from the top intake at the Lake Manassas dam.

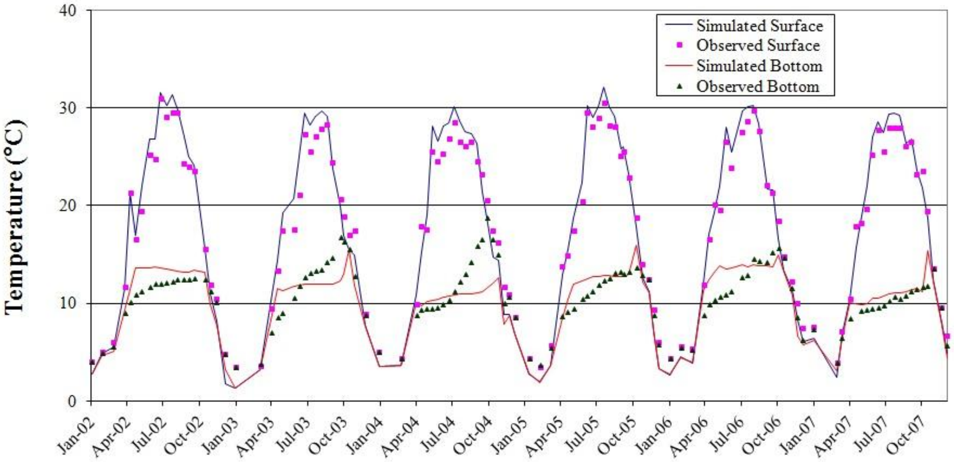


Figure 6-6: Comparison of Surface and Bottom Temperature at LM01 for Model Calibration (2002-2005) and Validation (2006-2007)

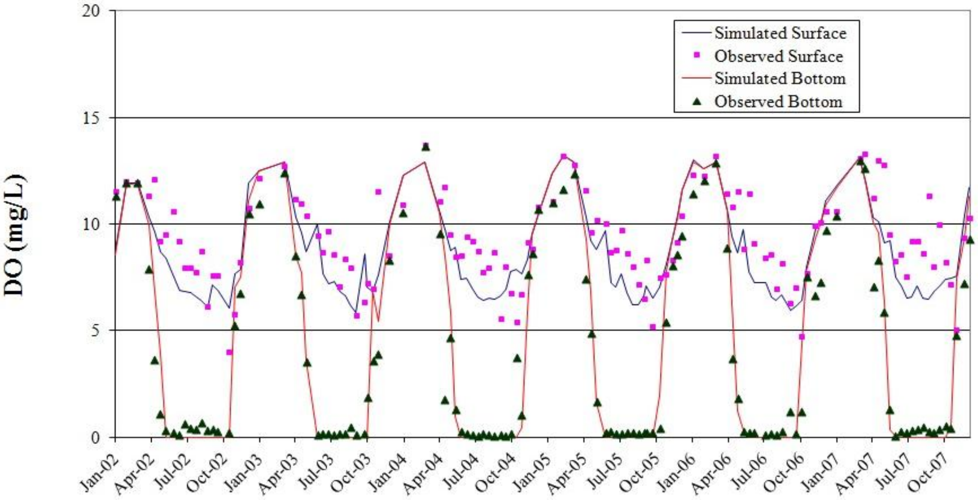


Figure 6-7: Comparison of Surface and Bottom DO Concentrations at LM01 for Model Calibration (2002-2005) and Validation (2006-2007)

The CE-QUAL-W2 model captured the seasonal patterns for temperature and DO concentrations at the surface layer in the lake quite well. As shown in Figures 6-6 and 6-7, the lowest DO concentrations during summers when temperature were highest and algae were most active were reproduced well. The model also reproduced the bottom oxygen patterns, such as the bottom oxygen depletion during summers and DO increase, from fall overturn.

Lake Manassas experiences summer stratification. Successful capture of the stratification is very important for further water quality simulation. Simulated temperature profiles for selected days in the summer (June, July and August, periods of strongest stratification) from 2002 to 2005 are presented in Figure 6-8. The model captured the summer stratification well, with AME values in the range of 0.43 ℃ ~1.80 ℃ during the calibration period (Figure 6-8 and Table 6-4). As shown in Table 6-4, the summer stratification was also validated from 2006 to 2007, and relatively larger AME values were found from 0.81 ℃ to 2.57 ℃. Most discrepancies were because of over-prediction of temperatures in lower layers.

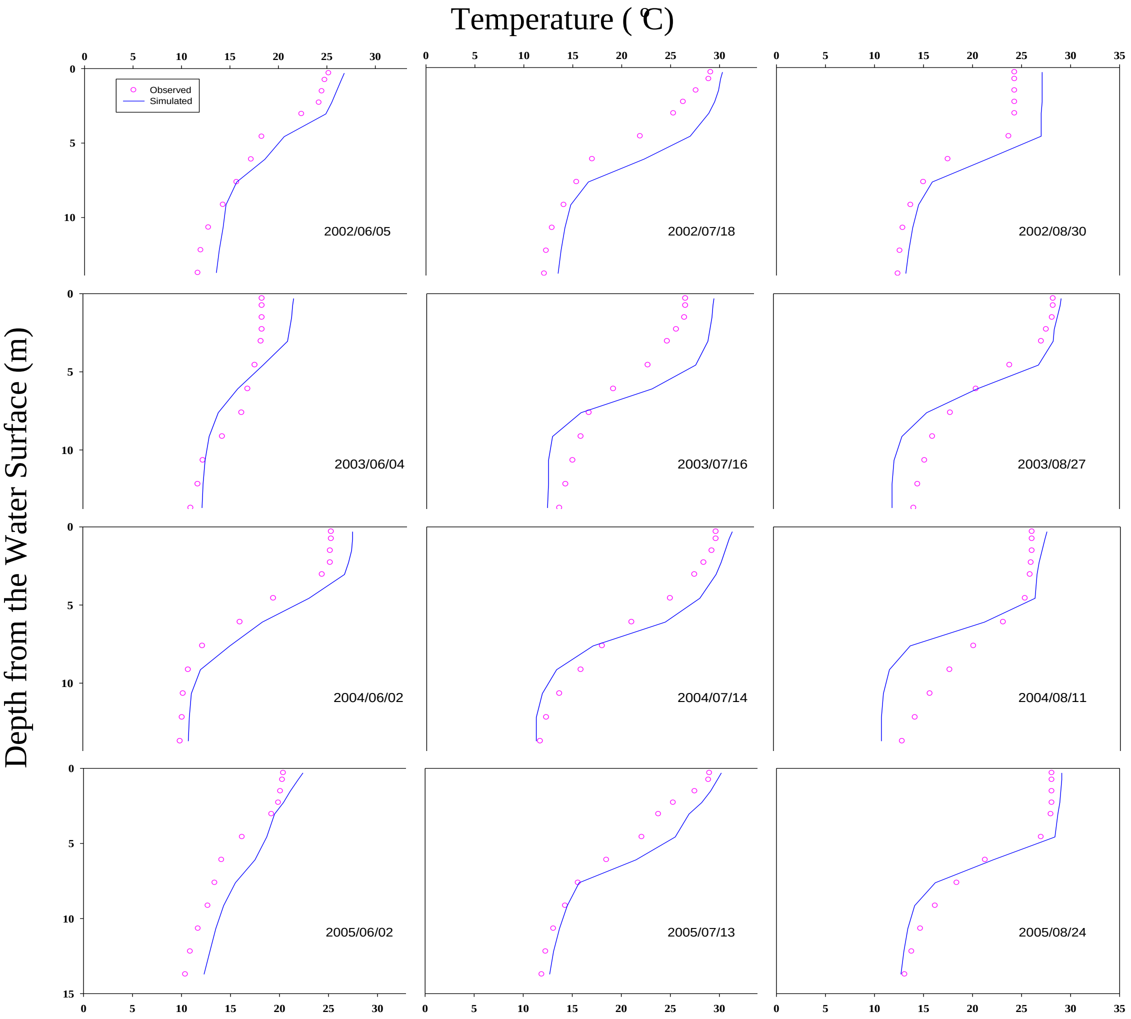


Figure 6-8: Comparison of Vertical Temperature Profile at LM01 near Lake Manassas Dam for the Calibration Period

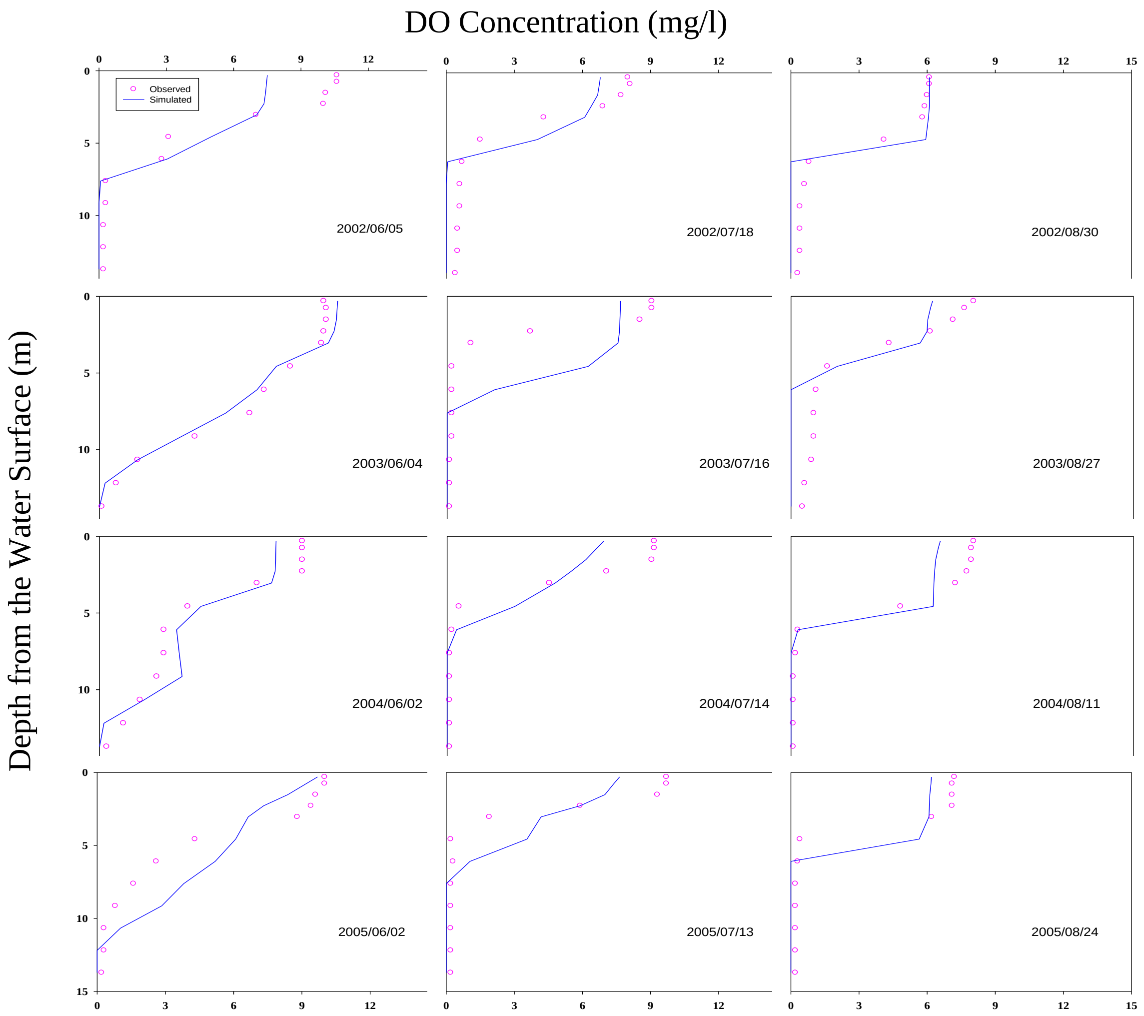


Figure 6-9: Comparison of Vertical DO Profile at LM01 near Lake Manassas Dam for the Calibration Period

The vertical distributions of DO concentrations were also captured for summer months. As shown in Figure 6-9, the oxygen depletion in the hypolimnion was well reproduced by the CE-QUAL-W2 model. However, differences between observed and simulated values were somewhat large in the upper layer (epilimnion), which are possibly related to algal activity. The DO AME values during the calibration period ranged from 1.12 mg/L to 2.75 mg/L (Table 6-4) and most discrepancies were due to the under-prediction of DO concentrations in the upper layer.

Table 6-4: Statistical Analysis of Summer Temperature and DO Concentrations at LM01 near Lake Manassas Dam

Date	Temperature		DO	
	AME	RMS	AME	RMS
06/05/2002	1.24	1.77	1.49	1.64
07/18/2002	0.97	1.15	2.34	2.80
08/30/2002	0.44	0.65	2.13	2.39
06/04/2003	0.43	0.50	1.79	2.06
07/16/2003	1.80	2.78	2.75	2.96
08/27/2003	0.95	1.06	1.70	2.01
06/02/2004	0.76	0.83	1.85	2.02
07/14/2004	1.01	1.47	1.72	1.90
08/11/2004	0.74	0.99	2.56	3.24
06/02/2005	1.37	1.60	1.73	1.91
07/13/2005	1.17	1.64	1.56	1.94
08/24/2005	0.88	1.63	1.12	1.23
06/01/2006	2.57	3.43	1.87	2.02
07/12/2006	0.81	1.46	1.25	1.40
08/23/2006	1.11	1.70	1.28	1.55
06/06/2007	1.54	1.95	1.53	1.56
07/18/2007	1.58	2.11	1.76	2.58
08/29/2007	1.97	2.69	0.69	0.89

Water Quality Simulation

Table 6-5 includes the comparison of average surface and bottom nutrient (OP, NH_4-N and Ox-N) concentrations at the five lake stations. Further analysis results at LM01 near the Lake Manassas dam are shown in Figures 6-10, 6-11 and 6-12.

As shown in Table 6-5, absolute differences between simulated and observed average surface OP concentrations were equal to or less than 0.004 mg/l at various lake stations during both calibration and validation periods. The differences in the bottom layers were relatively large especially at LM01 (+0.012 mg/l for calibration and −0.015 mg/l for validation). This might be related to bottom OP release under anoxic hypolimentic conditions, which is more likely to happen in lacustrine zones than riverine zones. As shown in Figure 6-10, the CE-QUAL-W2 model captured the OP seasonal trends in the lake, and the highest bottom concentrations were found during the summers. Although the timing of bottom OP release was generally captured, the model over-predicted bottom

OP concentrations in 2002 and 2003 but under-predicted some high OP concentrations from 2005 to 2007.

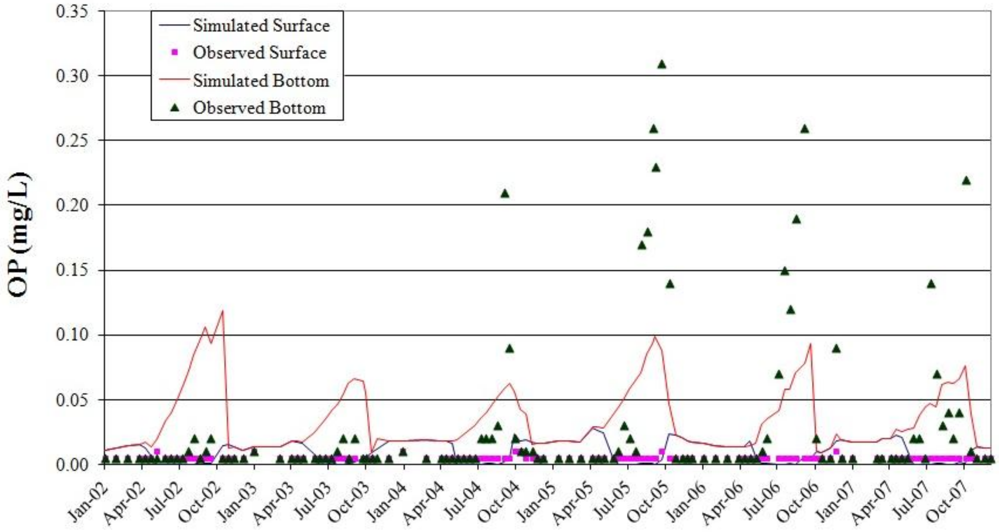


Figure 6-10: Comparison of Surface and Bottom OP Concentrations at LM01 for Model Calibration (2002-2005) and Validation (2006-2007)

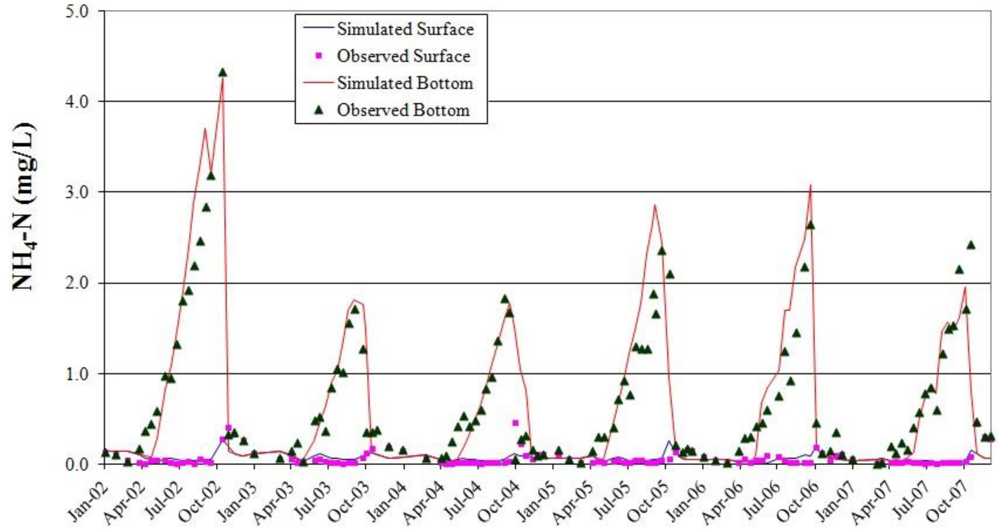


Figure 6-11: Comparison of Surface and Bottom NH_4-N Concentrations at LM01 for Model Calibration (2002-2005) and Validation (2006-2007)

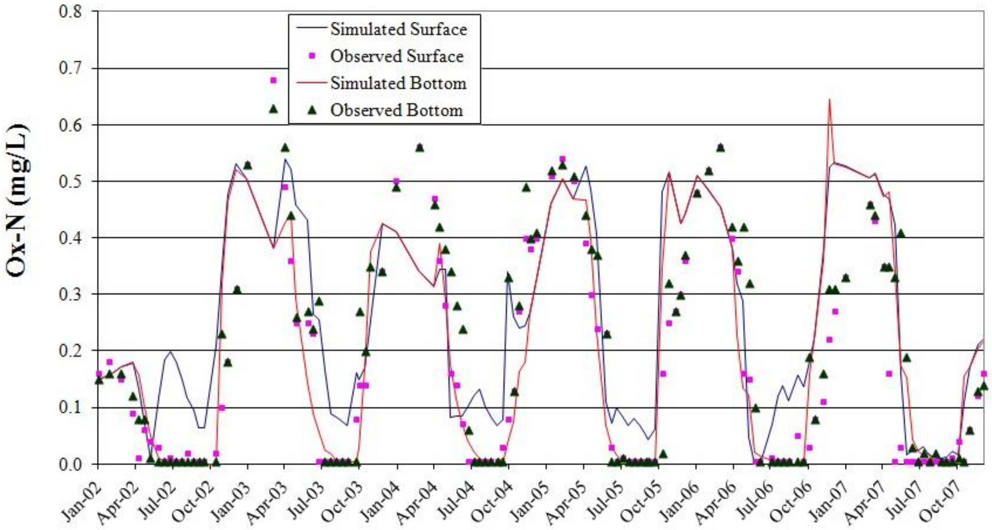


Figure 6-12: Comparison of Surface and Bottom Ox-N Concentrations at LM01 for Model Calibration (2002-2005) and Validation (2006-2007)

Figures 6-11 and 6-12 show that the CE-QUAL-W2 model reproduces the temporal distribution of NH_4-N and Ox-N concentrations very well. Both timing and magnitude of the seasonal nitrogen cycle at surface and bottom layers were well simulated.

Table 6-5: Comparison between Simulated and Observed Nutrient (OP, NH$_4$-N and Ox-N) Concentrations at Lake Manassas Stations

		LM01	LM03	LM04	LM05	LM06
				OP (mg/l)		
Surface	Observed	0.005/0.005*	0.005/0.006	0.005/0.005	0.006/0.005	0.006/0.005
	Simulated	0.009/0.009	0.009/0.008	0.009/0.008	0.008/0.008	0.008/0.009
	Difference	**0.004/0.004**	**0.004/0.002**	**0.004/0.003**	**0.002/0.003**	**0.002/0.004**
Bottom	Observed	0.027/0.049	0.006/0.007	0.014/0.023	0.006/0.009	0.007/0.005
	Simulated	0.039/0.034	0.021/0.017	0.028/0.026	0.017/0.016	0.009/0.009
	Difference	**0.012/–0.015**	**0.015/0.010**	**0.014/0.003**	**0.011/0.007**	**0.002/0.004**
				NH$_4$-N (mg/l)		
Surface	Observed	0.068/0.063	0.073/0.050	0.066/0.055	0.055/0.043	0.046/0.041
	Simulated	0.072/0.051	0.074/0.055	0.069/0.049	0.067/0.046	0.062/0.044
	Difference	**0.004/–0.012**	**0.001/0.005**	**0.003/–0.006**	**0.012/0.003**	**0.016/0.003**
Bottom	Observed	0.782/0.692	0.152/0.125	0.468/0.397	0.154/0.141	0.098/0.061
	Simulated	0.864/0.657	0.207/0.108	0.457/0.324	0.176/0.129	0.062/0.044
	Difference	**0.082/–0.035**	**0.055/–0.017**	**–0.009/–0.073**	**0.022/–0.012**	**–0.036/–0.017**
				Ox-N (mg/l)		
Surface	Observed	0.168/0.137	0.162/0.128	0.170/0.136	0.183/0.148	0.214/0.172
	Simulated	0.236/0.220	0.239/0.212	0.237/0.221	0.241/0.229	0.259/0.262
	Difference	**0.068/0.083**	**0.077/0.084**	**0.067/0.085**	**0.058/0.081**	**0.045/0.090**
Bottom	Observed	0.194/0.185	0.192/0.167	0.219/0.197	0.228/0.180	0.288/0.223
	Simulated	0.172/0.202	0.247/0.244	0.200/0.223	0.269/0.242	0.291/0.278
	Difference	**–0.022/0.017**	**0.055/0.077**	**–0.019/0.026**	**0.041/0.062**	**0.003/0.055**

*Calibration value/validation value

The calibration and validation results at various lake stations indicate that the CE-QUAL-W2 model captured spatial trends of NH$_4$-N concentrations fairly well. The average concentrations of NH$_4$-N tend to be similar among different stations in the surface layers, which were captured well by the model. At the five stations, the absolute differences between simulated and observed surface NH$_4$-N concentrations were equal to or less than 0.016 mg/L during both calibration and validation periods. In the bottom layers, the average NH$_4$-N concentrations tend to increase toward the dam, from the lowest level at LM06 (headwater) to the highest level at LM01 (near dam). CE-QUAL-W2 captured this spatial trends too, although the differences at the bottom layers are relatively large, with ranges of −0.009 mg/L ~ +0.082 mg/L during the calibration period and −0.017 mg/L ~ −0.073 mg/L during the validation period.

Surface Ox-N concentrations were generally over-predicted at various lake stations, probably due to over-prediction in the HSPF/AGCHEM models, which generated inputs for the CE-QUAL-W2 model (Table 6-5 and Figure 6-12). Bottom Ox-N concentrations were reproduced fairly well. At various lake stations, differences between observed and simulated bottom Ox-N concentrations were in the range of –0.019 mg/L ~ +0.055 mg/L during the calibration period and +0.017 mg/L ~ +0.077 mg/L during the validation period.

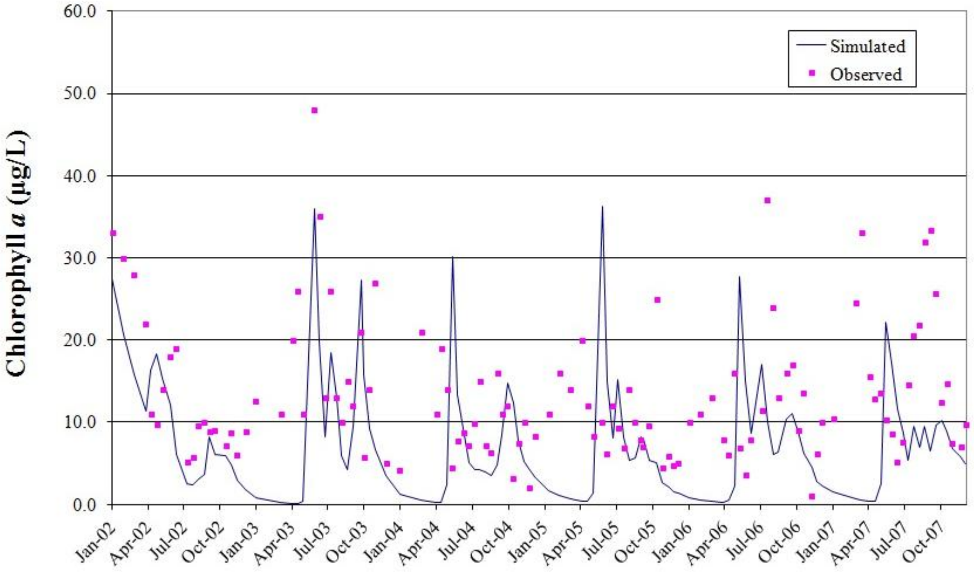


Figure 6-13: Comparison of Chl *a* Concentrations at LM01 for Model Calibration (2002-2005) and Validation (2006-2007)

Figure 6-13 shows a fair match between simulated and observed chl *a* concentrations at LM01. Chl *a* is an indicator of algae growth, which is an important component in the water quality model due to its interaction with nutrients and DO. As can be seen, the CE-QUAL-W2 model reproduced algae blooms well during the summers.

6.4.2 Pre-BMP Scenario Analysis Results

As described earlier, the N and P fertilizer application rates in the pre-BMP scenario were set to be the product of the current application rates and the corresponding application adjustment factors: 1.1 for N fertilizer and 1.75 for P fertilizer. As expected, NH_4-N and Ox-N loads from the Upper Broad Run subbasin didn't change much under the pre-BMP scenario (Table 6-6). The average annual OP load increased by 79.6% if the pre-BMP fertilizer application rate was used. The largest increase of the OP loads is in spring (Figure 6-14), as most P fertilizer is applied in that season.

Table 6-6: Average Annual Nutrient Loads for Upper Broad Run Subbasin under Current and Pre-BMP Scenarios

	Average Annual loads (10^6 g)		
	NH_4-N	Ox-N	OP
Current	2.77	36.73	0.81
Pre-BMP	2.86	38.46	1.45
Percent Difference (Pre-BMP - Current)	3.3%	4.7%	79.6%

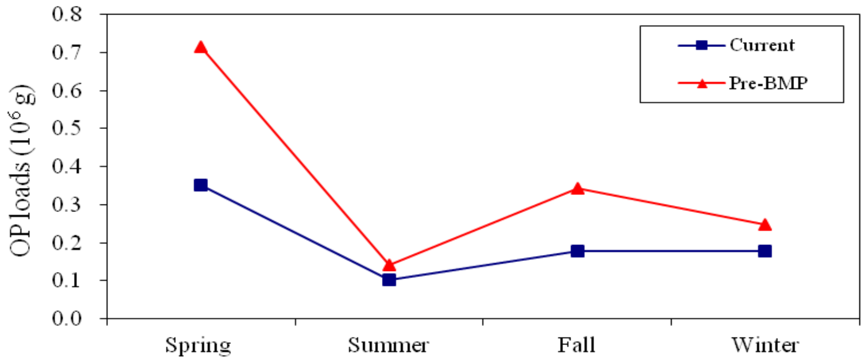


Figure 6-14: Seasonal OP Loads for Upper Broad Run Subbasin under Current and Pre-BMP Scenarios

In addition, increases of the OP yields were not evenly spread across the watershed. As shown in Figure 6-15, under the pre-BMP scenario, the OP yield increased more in the western part of the watershed, where there are more agricultural land uses. This indicates the effectiveness of implementing a nutrient management plan for NPS control in agriculturally dominated watersheds. For urban dominated watersheds, other BMPs might be better solutions to control NPS.

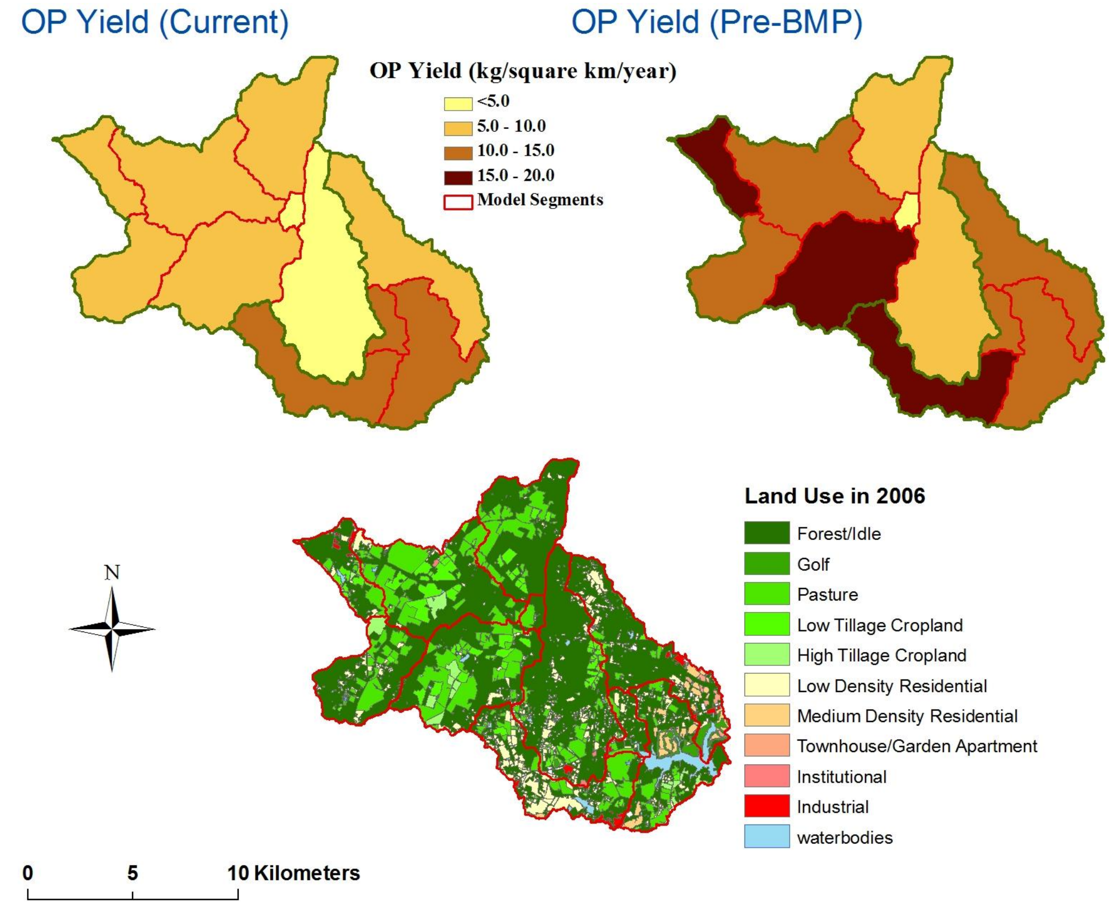


Figure 6-15: OP Yields in the Lake Manassas Drainage Areas under Current and Pre-BMP Scenarios

Table 6-7: Average Water Quality Concentrations at LM01 under Current and Pre-BMP Scenarios

	NH_4-N (mg/l)		Ox-N (mg/l)		OP (mg/l)		Chl *a* (µg/l)
	Surface	Bottom	Surface	Bottom	Surface	Bottom	
Current	0.068	0.864	0.227	0.172	0.009	0.039	8.062
Pre-BMP	0.069	0.869	0.236	0.178	0.014	0.049	10.052
Percent Difference (Pre-BMP - Current)	0.7%	0.5%	3.7%	3.5%	54.7%	25.0%	24.7%

In response to the increased OP loads from the watershed under the pre-BMP scenario, surface and bottom OP concentrations at station LM01 (nearest the Lake Manassas dam) increased by 54.7% and 25.0% respectively (Table 6-8). Without the nutrient management plan, the pre-BMP scenario would increase average chl *a* concentrations by 24.7%. As shown in Figures 6-18 and 6-19, the average OP and chl *a* concentrations also increased at other stations along the mainstem of Lake Manassas. These increases at LM04, LM05 and LM06, the latter of which is just downstream of where Broad Run drains into Lake Manassas, were similar to those at LM01. This indicates that the increases of external OP loads not only result in OP enrichment of the lake, but also stimulate algae growth.

Despite a significant increase of OP loads in spring, the OP concentration increase under the pre-BMP scenario didn't show a significant seasonal trend (Figure 6-16). On the other hand, algae growth (represented as chl *a*) due to excess OP loads showed the greatest increase in summer (Figure 6-17).

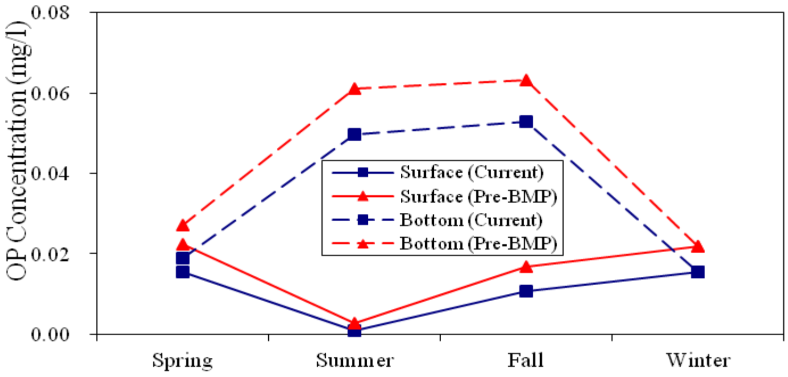


Figure 6-16: Seasonal OP Concentration at LM01 under Current and Pre-BMP Scenarios

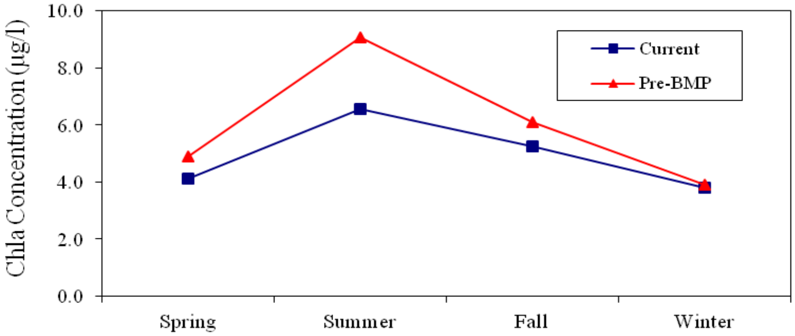


Figure 6-17: Seasonal Chl *a* Concentration at LM01 under Current and Pre-BMP Scenarios

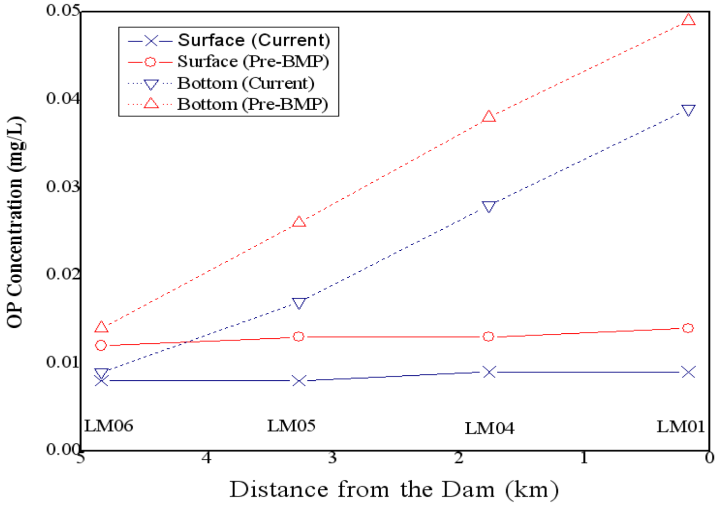


Figure 6-18: Comparison of Spatial Distribution of OP concentrations along the Mainstem of Lake Manassas under Current and Pre-BMP Scenarios

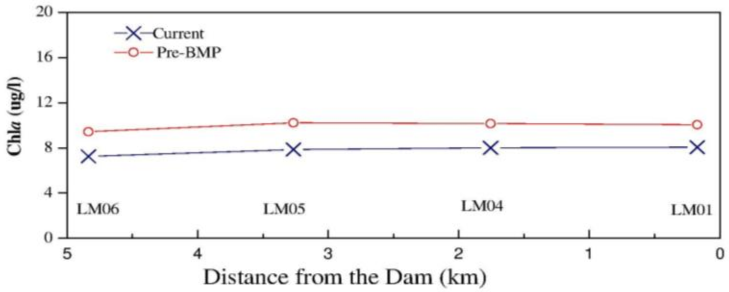


Figure 6-19: Comparison of Spatial Distribution of Chl *a* Concentrations along the Mainstem of Lake Manassas under Current and Pre-BMP Scenarios

6.5 Conclusions

The HSPF/AGCHEM model applications for the Upper Broad Run and Middle Broad Run subbasins were considered to generate good flow and pollutant inputs for Lake Manassas CE-QUAL-W2 model. The calibration (2002-2005) and validation (2006-2007) results indicate that the CE-QUAL-W2 model adequately captured water surface elevation, temperature, DO concentration, temporal and spatial variations of nutrient (NH_4-N, Ox-N, and OP) concentrations, as well as chl *a* concentration in Lake Manassas.

The study also demonstrates the application of HSPF/AGCHEM within a linked watershed-reservoir model to evaluate a nutrient management plan implementation in the Lake Manassas watershed. The evaluation was based on the current simulation and a pre-BMP scenario. In the current simulation, N and P fertilizer applications were based on the recommendations of Virginia Cooperative Extension considering nutrient management plan. The pre-BMP scenario was designed to represent N and P fertilizer application rates 20 years ago, which were estimated to be 110% of the current N and 175% of the current P application rates. The fertilizer applications in the current condition and pre-BMP scenario were incorporated into the Upper Broad Run and Middle Broad Run HSPF/AGCHEM models, so that the CE-QUAL-W2 model used the boundary conditions corresponding with the two scenarios to predict water quality benefits of implementing the nutrient management plan.

The pre-BMP scenario analysis results demonstrate the capabilities of the linked model to develop a direct cause-and-effect relationship between watershed nutrient management and downstream water quality in the receiving waterbody. Without the nutrient management plan, the average annual OP load from the Upper Broad Run subbasin would have increased by 79.6%. The increase of external OP loads would have lead to accumulation of OP in the Lake Manassas, and OP concentrations would have increased by 54.7% and 25% at surface and bottom layers, respectively. The higher OP concentrations would have stimulated algae growth (represented as a 24.7% increase of chl *a* concentration) and worsen the water quality issues. This indicated that implementing the nutrient management plan in the Lake Manassas watershed played an important role in reducing the nutrient enrichment and eutrophication condition of the lake. Another finding from the study is that the increases of the OP yields without the nutrient management plan would have been more apparent in agricultural intensive areas, thus indicating the effectiveness of implementing nutrient management plans for NPS control in agriculturally dominated watersheds.

6.6 References

Bicknell, B.R., Imhoff, J.C., Kittle, J.L., Jobes, T.H., and Donigian, A.S, 2005. Hydrological Simulation Program -Fortran (HSPF). User's manual for release 12.2. U.S.EPA. National Exposure Research Laboratory, Athens, GA.

Borah, D. K., and Bera, M., 2004. Watershed-scale hydrologic and nonpoint-source pollution models: Review of applications. Trans. ASAE 47(3): 789-803.

Bouraoui, F., and Dillaha, T. A., 2000. Answers-2000: Nonpoint source nutrient planning model. J. Environ. Eng. 126: 1045-1055.

Burgholzer, R., 2007. Report of a Workshop on Understanding Fertilizer Sales and Reporting Information. U.S. EPA Chesapeake Bay Program Scientific and Technical Advisory Committee and the Agricultural Nutrient Reduction Workgroup. U.S. EPA, Washington, DC.

Chesapeake Bay Program Office (CBPO), 2004. Tributary Strategy Tool. Available at http://www.chesapeakebay.net/tribtools.htm. Accessed 30 July, 2007.

Cole, T. M., and Wells, S. A., 2008. CE-QUAL-W2: A Two-Dimensional, Laterally Averaged, Hydrodynamic and Water Quality Model, Version 3.6 User Manual. In. Washington, DC: U.S. Army Corps of Engineers.

Debele, B., Srinivasan R., and Parlange. J. Y., 2006. Coupling upland watershed and downstream waterbody hydrodynamic and water quality models (SWAT and CE-QUAL-W2) for better water resources management in complex river basins. Environ Model Assess.

DePinto, J.V., Freedman, P.L., Dilks, D.M., and Larson, W.M., 2004. Models Quantify the Total Maximum Daily Load Process. Journal of Environmental Engineering, 130(6), 703-713.

Donigian, A. S., Bicknell, B. R., Patwardham, A. S., Linker, L. C., and Chang, C., 1994. Chesapeake Bay Program: watershed model application to calculate bay nutrient loadings. U.S. EPA-903-R-94-042, Chesapeake Bay Program Office. U.S.EPA. Annapolis, Maryland.

Eggink, J., 2001. An Exploration of the Limnological Dynamics of Lake Manassas. Master's Thesis, Virginia Polytechnic Institute and State University, Falls Church, Virginia.

Flowers, J. D., Hauck, L. M., and Kiesling, R., 2001. USDA: Lake Waco-Bosque River Initiative: Water Quality Modeling of Lake Waco Using CE-QUAL-W2 for Assessment of Phosphorus Control Strategies, Texas.

Gorrie, J.R., 2007. An Examination Of Water Quality Impacts On Lake Manassas. Master Thesis, Virginia Polytechnic Institute and State University, Falls Church, Virginia.

Im, S., Brannan, K.M., and Mostaghimi, S., 2003. Simulating Hydrology and Water Quality Impacts in an Urbanizing Watershed. JAWRA 39(6): 1465-1479.

Liu, Z., Kingery, W.L., Huddleston, D. H., Hossain, F., Hashim N. B., and Kieffer J. M., 2008. Application and evaluation of two nutrient algorithms of Hydrological Simulation Program Fortran in Wolf River watershed. Journal of Environmental Science and Health, Part A 43(7):738-48.

Liu, Y., Godrej, A.N., and Grizzard, T.J., 2011a. Sensitivity Analysis, Calibration and Validation of a Watershed Model Application using HSPF with the Nutrient Algorithm PQUAL in Upper Broad Run Watershed, Virginia. In Submission.

Liu, Y., Godrej, A.N., Grizzard, T.J., and Dillaha, T. A., 2011b. Application and Sensitivity Analysis of a Watershed Model Application using HSPF with the Nutrient Algorithm AGCHEM in Upper Broad Run Watershed, Virginia. In Submission.

Marshall, J., 2009. Personal Communication. Fauquier County Soil and Water Conservation District, Virginia.

Neitsch, S.L., Arnold, J.R., Kiniry, J.R., Williams, J.R., and King, W.K., 2002. Soil and Water Assessment Tool Theoretical Documentation Version 2000. Texas Water Resources Institute, College Station, Texas.

Ohlwiler, T., 2009. Personal Communication. Fauquier County Cooperative Extension Office, Virginia.

Saleh, A., and Du, B., 2004. Evaluation of SWAT and HSPF within BASINS Program for the Upper North Bosque river watershed in Central Texas, Transactions of the ASAE Vol. 47(4): 1039-1049.

U.S. Department of Agriculture (USDA), 2004. National Agricultural Statistics Service. 2002 census of agriculture. Available at http://www.nass.usda.gov/census.

United States Environmental Protection Agency (USEPA), 2002. National Water Quality Inventory 2000 Report. EPA-841-R-02-001, Washington, DC.

U.S. Natural Resources Conservation Service (NRCS), 2006. National Conservation Practice Standard: Nutrient Management. Code 590, Fort Worth, TX.

Virginia Department of Conservation and Recreation (VDCR), 2005. Virginia Nutrient Management Standards and Criteria.

Wool, T. A., Ambrose, R. B., Martin, J. L., and Cormer, E. A., 2003. Water Quality Analysis Simulation Program (WASP) Version 6.0 Draft: User's Manual. In. Atlanta, Georgia: U.S. Environmental Protection Agency.

Wu, J., 2004. Water-quality-based BMP design approach and uncertainty analysis for integrated watershed management. PhD. Dissertation, University of Virginia.

Xu, Z., 2005. A complex, linked watershed-reservoir hydrology and water quality model application for the Occoquan Watershed, Virginia. PhD. Dissertation, Virginia Tech.

Young, R.A., Onstad, C.A., Bosch, D.D., and Anderson, W.P., 1994. Agricultural Non-Point Source Pollution Model, Version 4.03 AGNPS User's Guide. U.S. Department of Agriculture, Washington, D.C.

Chapter 7. Evaluating HSPF Performance of Flow and Sediment Prediction at Multiple Watershed Segmentations in Upper Broad Run Watershed, Virginia

Yingmei Liu[1], Adil N. Godrej[2], and Thomas J. Grizzard[3]
[1]*PhD graduate, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*
[2]*Research Associate Professor, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*
[3]*Professor, Civil and Environmental Engineering, Virginia Tech, Manassas, VA*

To be submitted to ASCE, *Journal of Hydrologic Engineering*

7.1 Abstract

The popular watershed model HSPF is being widely used as a convenient means of predicting the hydrology and water quality impacts associated with climate, land use and management change. Model calibration with respect to local observed data is typically used to improve model predictability. However, a significant concern is how well the calibrated model performs in a predictive mode. In this paper, HSPF applications in the Upper Broad Run watershed in Northern Virginia calibrated from 1993 to 1997 at a coarser segmentation and calibrated from 2002 to 2007 at a finer segmentation were used in a predictive manner for time periods with available data to assess HSPF performance of flow and sediment prediction. The Upper Broad Run, located in the larger Occoquan watershed in Virginia, is a rural watershed undergoing continuous urbanization. It was found that HSPF was able to predict reasonable good flows at both watershed segmentations when extended 10 years beyond the calibration period. However, both applications generally underestimated sediment loadings, indicating that appropriate judgment should be exercised when using the applications for sediment prediction.

In addition, the HSPF applications at the two segmentations were compared to investigate segmentation effect on simulated flow and sediment discharges. Compared to the HSPF

application at the coarser segmentation, the HSPF application at the finer segmentation didn't show improvement in flow simulation but showed noticeable improvement for sediment simulation.

7.2 Introduction

The Hydrological Simulation Program-FORTRAN (HSPF) is one of the most extensively used watershed hydrology and water quality models for long–term continuous simulations in mixed agricultural and urban watersheds (Borah and Bera, 2003). There have been many hundreds of applications of HSPF in different geographic regions all over the world (for example, Diaz-Ramirez et al., 2008; Mishra et al., 2007; Hayashi et al., 2001). One of the largest applications of HSPF is to determine total watershed contributions of flow, sediment and nutrients from the 64,000 square mile Chesapeake Bay watershed (Donigian et al., 1994; Donigian et al., 1998).

An important modeling purpose of HSPF applications is to develop a watershed model with predictive ability (Borah and Bera, 2004; Brun and Band, 2000; Laroche et al., 1996). Model calibration with respect to local observed data is typically used to improve model predictability. However, when a model has a large number of parameters to be calibrated, and the connection of these parameter values to physical processes is not straightforward, successful completion of a calibration can be quite challenging (Al-Abed and Whiteley, 2002). HSPF has many parameters and the calibration process can be a long one.

Model parameters estimated through calibration can be used in predicting future system behavior, such as under the influence of changed climate, and management of land use. A significant concern of those in planning and management of land use is how well the calibrated model performs in a predictive mode. Rahman and Salbe (1995) used HSPF to study the impact of urbanization and point-source pollution management scenarios on the South Creek catchment near Sydney, Australia, and acknowledged that authenticity of their results was unknown without model validation. Many watershed modeling studies (Donigian A. S., 2002; Xu et al., 2007; Singh et al., 2005) used a calibration-verification procedure for model validation, mostly with the same land use data for both the calibration and verification periods. One study in the Upper San Pedro watershed (Semmens et al., 2006) used a SWAT (Soil and Water Assessment Tool) model developed with historic data to conduct predictive “future” simulations for time periods with available data to assess SWAT performance for hydrologic prediction, which was considered as a forecasting validation. In the study, the forecasting validation reflected both climate and land use changes and provided an opportunity for a rigorous test.

HSPF application models typically subdivide a watershed into smaller segments. The individual segments are assumed to be homogeneous with respect to, among others, channel network, watershed topography, soil, land use, and climate inputs. HSPF is a lumped parameter model where parameter values are representative of the entire segment. Watershed segmentation issues have been addressed in many watershed modeling studies (Mamillapalli et al., 1996; FitzHugh and MacKay, 2000; Gong et al., 2010). Most studies were conducted for SWAT and found that simulated streamflow was insensitive to the number of segments but sediment yield estimates were relatively sensitive to watershed segmentation (Bingner et al., 1997; Jha et al., 2004; Arabi et al., 2006). Effects from different watershed segment sizes on a DWSM (dynamic watershed simulation model) input parameters and water and sediment discharges were investigated on the Big Ditch watershed (Borah et al., 2004). It was found from the study that three input parameters required recalibration when watershed segment sizes were altered and simulated water and sediment discharges were approximately same for both the coarser and finer segmentations. However, a literature review shows that few studies have been done on the effect of watershed segmentation in HSPF on simulated water and sediment discharge.

The principal objective of this paper was to evaluate HSPF performance with respect to flow and sediment prediction at multiple watershed segmentation levels. The study was conducted for the Upper Broad Run watershed which is located in the larger Occoquan watershed in Northern Virginia, and which is a rural watershed undergoing active urbanization. The base Upper Broad Run model applications used were part of the larger Occoquan watershed model for developed separately for various periods. The coarser (three segments) HSPF application in the Upper Broad Run watershed, calibrated for 1993-97, was used in a forward predictive manner to assess flow and sediment prediction performance for the time periods 1998-2001 and 2002-2007. The more finely segmented 2002-07 HSPF application (seven segments), was used in a backward predictive manner for the periods 1993-97 and 1998-2001. Basic data, such as meteorology and land use, were unchanged form that used for the three time periods. By evaluating how the coarser and finer segmentation model applications performed when extended approximately 10 years outside their calibration period under varying meteorology and land use conditions, it was expected that practitioners would obtain better guidance and more confidence in using the model as a prediction tool.

7.3 Study Site

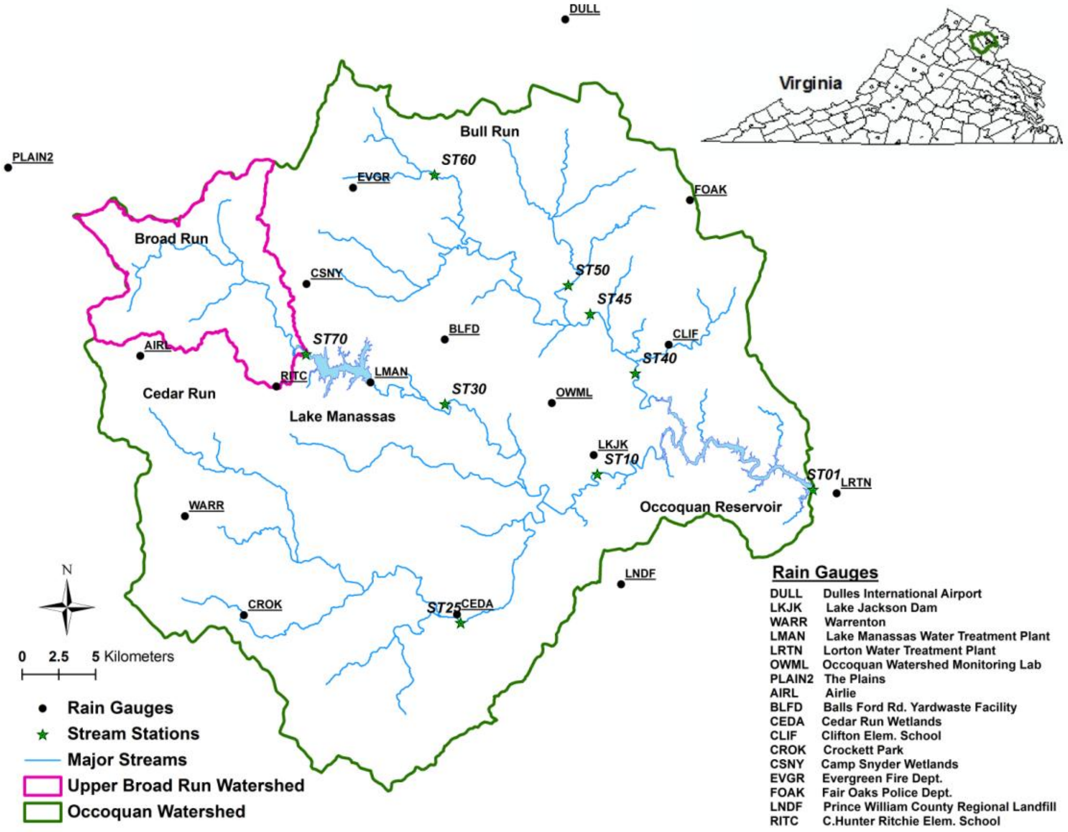


Figure 7-1: Location of Upper Broad Run Watershed, Showing Major Streams, Stream Stations and Rain Gauges in the Occoquan Watershed

The Upper Broad Run watershed is located in the Piedmont Region physiographic province, underlain by metamorphic rocks of diverse origins that can be traced back to the Paleozoic period (VDMR, 2001). Much of the study site falls into the Foothills subprovince, which has moderate slopes and relatively high elevation from 400 ft (121.92 m) to 1000 ft (304.8 m). The soils are generally loam and moderately well-drained. Based on the information from the State Soil Geographic (STATSGO) database, about 67% of the soils are categorized as B for the SCS (Soil Conservation Society) hydrological soil group, which features a moderate infiltration rate when thoroughly wetted. Upper Broad Run is a rural watershed that is undergoing continuous urbanization.

7.4 Model Description and Methods

7.4.1 Brief Description of HSPF

HSPF is a comprehensive, continuous, conceptual lumped model designed to simulate hydrology and water quality processes in a watershed (Bicknell et al., 2005). It is included within the US Environmental Protection Agency (EPA) Better Assessment Science Integrating Point and Nonpoint Sources (BASINS) package.

HSPF consists of three application modules—PERLND, IMPLND, and RCHRES—which simulate runoff and water quality constituents from pervious and impervious lands, and free flow reaches/well-mixed impoundments, respectively. Bicknell et al. (2005) and Donigian et al. (1995) provide detailed descriptions of these modules. The flow and sediment simulations with these modules, which are of primary interest to this study, are briefly described below.

Flow simulation

HSPF simulates a complete land-side water budget on pervious and impervious lands separately. On pervious lands, water budget considers evapotranspiration, soil moisture storage, deep percolation, and outflows (as surface runoff, interflow, and groundwater) in response to precipitation and snowmelt. Each of the allocations can be controlled with parameters describing infiltration-excess process and storage-capacity factors represented by empirical equations. Impervious lands, where no infiltration occurs, principally generate surface runoff. Water from surface runoff, interflow, and groundwater continues to be routed in the streams by use of storage-volume relationships (Bicknell et al., 2005).

Sediment simulation

HSPF simulates overland sediment erosion and transport by using exponential relationships for soil detachment and washoff. In-stream sediment deposition, scour and transport are simulated in three classes: sand, silt, and clay.

Non-cohesive (sand) sediment transport can be simulated based on a sand-carrying capacity of the stream as a power function of the average flow velocity. Sand that exceeds the capacity will be deposited, and sand below the capacity will be scoured. Cohesive (silt, clay) sediment transport can be simulated based on a bed shear stress as a function of the slope and hydraulic radius of the stream. Sediment will be scoured if the bed shear stress is above a specified critical shear stress for scouring, and deposited if the bed shear stress is below a specified critical shear stress for deposition (Bicknell et al., 2005).

7.4.2 HSPF Applications in the Upper Broad Run Watershed

The Upper Broad Run watershed was simulated with HSPF in the larger complexly-linked watershed-reservoir model for the Occoquan watershed. The complete linked Occoquan model was developed and calibrated for a simulation period 1993-1997 (Xu, 2005). Because HSPF does not allow land use changes during a simulation period, the simulation periods we used (1993-97, 1998-2001, 2002-07) bracketed the observed land use data (1995, 2000 and 2006, respectively).

Watershed segmentation

In 2001, additional new rain gauge stations (Figure 7-1) were established in the Occoquan Watershed to provide more precipitation coverage than previously available. Due to the availability of additional precipitation data, a finer segmentation was performed on the Occoquan watershed for the simulation period 2002-07. The automatic delineation tool of BASINS was used to delineate the watershed and subdivide it into model segments. The automatic delineation tool allowed a delineation of the watershed based on a DEM elevation file, NHD stream network data, and user defined threshold area (minimum size of segments), providing fast results and reducing uncertainty during the delineation process.

The Upper Broad Run watershed at the coarser segmentation (with a threshold area of 15 km^2) and the finer segmentation (with a threshold area of 7.5 km^2) is shown in Figure 7-2. Some of the segment and reach characteristics are summarized in Table 7-1.

Table 7-1: **Segment and Reach Characteristics of the Upper Broad Run Watershed at the Coarser and Finer Segmentation**

	Coarser segmentation	Finer segmentation
Number of segments	3	7
Average segment size (km^2)	42.07	18.03
Average elevation (m)	524.00	580.71
Average slope (%)	34.90	34.67
Average reach length (km)	8.67	5.43
Average reach slope (%)	5.20	7.53
Average reach width (m)	11.90	6.97
Average reach depth (m)	0.60	0.39

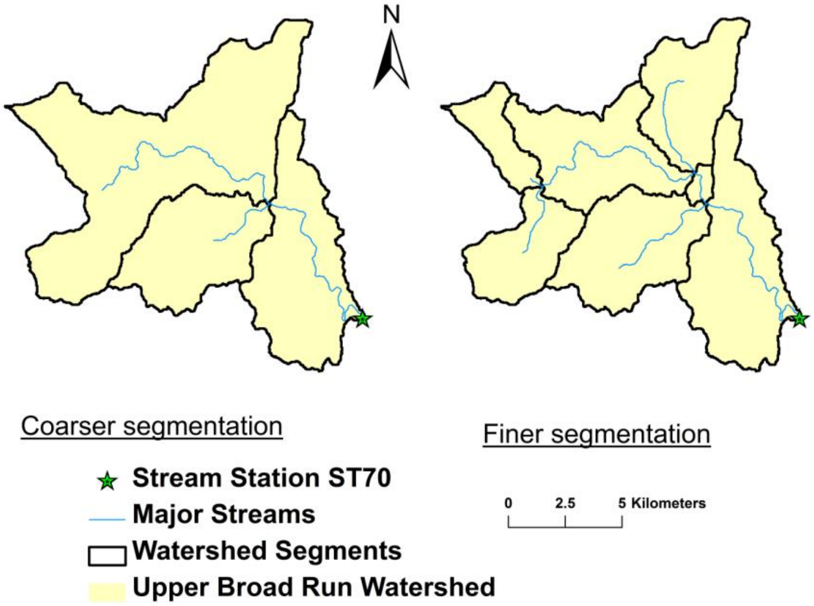


Figure 7-2: The Upper Broad Run Watershed at the Coarser and Finer Segmentation

Data sources

Input data needs for HSPF are extensive, including meteorological time series, and physical watershed-specific data (parameters that describe topographic, geometry and land use characteristics). In this study, the topographical and channel geometry data were transferred from BASINS to HSPF to be used either directly (i.e. FTABLEs) or indirectly (i.e. LSUR and SLSUR), as guided by BASINS Technical Note 6 (USEPA, 2000).

Land use data were obtained from the Northern Virginia Regional Commission (NVRC), which determines land use every five to six years by reducing aerial photography. Land use data were consolidated into nine land use categories to be simulated in the HSPF applications: forest, pasture, high tillage cropland, low tillage cropland, townhouse/garden apartment, low density residential, medium density residential, industrial/commercial, and institutional (Xu et al., 2007). The categorization was based on land imperviousness and soil characteristics. Based on the land use summary in 1995, 2000, and 2006 (Figure 7-3), Upper Broad Run is a rural watershed, with the urban area, including industrial, institutional, and low density residential, increasing. It should be noted that the increased forest/idle land use from 2000 to 2006 is because of different classification methods used by the NVRC for those years.

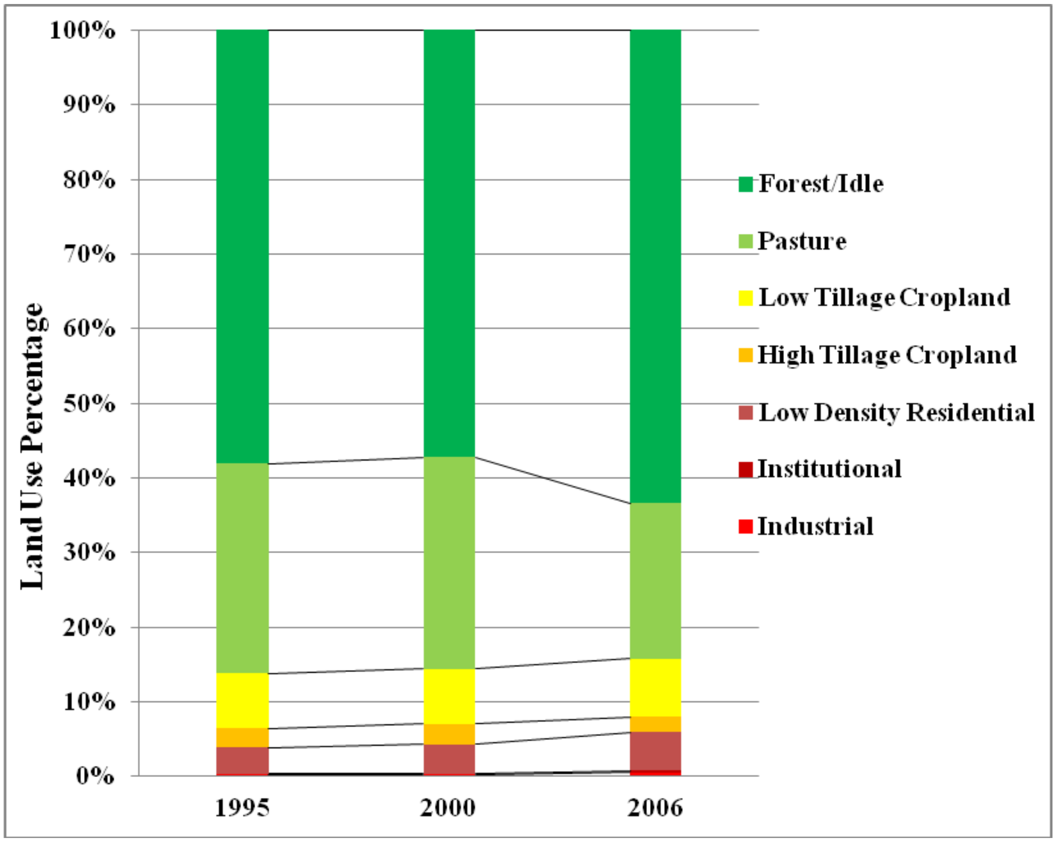


Figure 7-3: Land Use Proportions in the Upper Broad Run Watershed in 1995, 2000, and 2006

The meteorological data used by HSPF are air temperature, cloud cover, dew point temperature, potential evapotranspiration (ET), solar radiation, wind speed, and precipitation. Except for precipitation, all other meteorological data were obtained as hourly time series from the Washington Dulles International Airport weather station (DULL in Figure 7-1). Because potential ET data were not directly available from the Dulles station, the modified Penman Pan empirical method was used to estimate the potential ET from maximum daily air temperature, minimum daily air temperature, average daily dew point temperature, total daily wind movement and total daily solar radiation (Xu et al., 2007).

In the simulation periods of 1993-1997 and 1998-2001, hourly precipitation time series data from the Plains station (PLAIN2 in Figure 7-1) were used. Since the establishment of additional new rain gauge stations in the Occoquan watershed in 2001, precipitation data from AIRL (Airlie), RITC (C. Hunter Ritchie Elem. School), and CSNY (Camp Snyder wetlands) were used for the 2002-07 period. The new stations (except CSNY) provided the precipitation data at 10-minute intervals, which were aggregated to hourly average data to be used in this study. Daily data from station CSNY were disaggregated to hourly values based on hourly data distributions from neighboring stations.

Model calibration

Observed data from stream station ST70 (Figure 7-1) were used to calibrate the HSPF applications. Calibration for hydrology was followed by sediment calibration, and, lastly, water quality calibration (water quality results are not discussed here). Parameter selection and value ranges for the hydrology and sediment calibration were based on the guidance in BASINS technical notes (USEPA, 2000; USEPA, 2006). Values for the selected parameters were based on land use, agricultural activity, slope and soil characteristics, as well as literature values and previous local studies (Xu et al., 2007). During calibration, values were varied within recommended ranges to obtain a satisfactory agreement between simulated and observed flow and sediment loadings. The principal calibration parameters, recommended ranges, and calibrated values used in this study are listed in Table 7-2.

Table 7-2: Principal HSPF Calibration Parameters Used in this Study

Parameter	Definition	Recommended range* typical (possible)	Calibrated value (coarser segmentation)	Calibrated value (finer segmentation)
LZSN	Lower zone nominal storage	3.0-8.0 (2.0-15.0)	3.8	3.5
UZSN	Upper zone nominal storage	0.1-1.0 (0.05-2.0)	0.5-0.72†	0.4-0.62†
INFILT	Soil infiltration capacity index	0.01-0.25 (0.001-0.50)	0.13-0.18‡	0.13-0.18‡
LZETP	Lower zone ET parameter-an index to the density of deep rooted vegetation	0.2-0.7 (0.1-0.9)	0.46-0.8†	0.46-0.8†
INTFW	Interflow inflow parameter	1.0-3.0 (1.0-10.0)	3	3
IRC	Interflow recession parameter	0.5-0.7 (0.3-0.85)	0.5	0.5
AGWRC	Groundwater recession parameter	0.92-0.99 (0.85-0.999)	0.92	0.92
KRER	Coefficient in the soil detachment equation	0.15-0.45 (0.05-0.75)	0.45	0.45
JRER	Exponent in the soil detachment equation	1.5-2.5 (1.0-3.0)	2.5	2.0
KSER	Coefficient in the soil washoff equation	0.5-5.0 (0.1-10.0)	2.3-3.3‡	2.3-3.3‡
JSER	Exponent in the soil washoff equation	1.5-2.5 (1.0-3.0)	1.2	2.0
KSAND	Coefficient of sand load power function	0.01-0.5 (0.001-10.0)	0.1	0.1
EXPSND	Exponent of sand load power function	1.5-3.5 (1.0-6.0)	2	2
TAUCD (silt)	Critical bed shear stress for deposition (silt)	0.01-0.3 (0.001-2.0)	1.5	1.8
TAUCS (silt)	Critical bed shear stress for scour (silt)	0.05-0.5 (0.01-3.0)	1.8	2.1
M (silt)	Erodibility coefficient (silt)	0.01-2.0 (0.001-5.0)	0.1	0.1
TAUCD (clay)	Critical bed shear stress for deposition (clay)	0.01-0.3 (0.001-2.0)	1.5	1.8
TAUCS (clay)	Critical bed shear stress for scour (clay)	0.05-0.5 (0.01-3.0)	1.8	2.1
M (clay)	Erodibility coefficient (clay)	0.01-2.0 (0.001-5.0)	0.1	0.1

*Based on USEPA (2000), USEPA (2006)
†Varying by month and land use
‡Varying by land use

7.4.3 Model Performance Evaluation of Flow and Sediment Simulation

Two tests were designed for the evaluation of predictive (backward and forward) abilities of the 1993-97 and 2002-07 applications. These are described below. In both cases, observed data from the time periods were used to assess model performance.

Test1: The Upper Broad Run watershed model with the coarser segmentation (3 segments), calibrated for 1993-1997, was used to predict for the 1998-2001 and 2002-2007 periods. Meteorology and land use data for those periods were used, but parameter values and segmentation remained unchanged. Essentially, this process used the 1993-97 model with the coarser segmentation to predict 10 years beyond the calibration period.

Test2: The finer segmentation model (7 segments) for 2002-2007 was used to predict for the 1993-1997 and 1998-2001 periods. As in Test1, meteorology and land use data from the periods being simulated were used, whereas parameter values and segmentation were kept unchanged. This resulted in a backward prediction (sometimes also called a backcast) for the 10 years prior to the calibration period.

For each test, comparisons between observed and simulated flows and sediment loadings were used in model performance evaluation. Comparisons of monthly, annual and long term performance were evaluated using both statistical and graphical measures. Statistical measures of agreement included percentage difference (PD) for annual and long term data, and standard coefficient of determination (R^2) and Nash-Sutcliffe model efficiency (NSE) for monthly data. The percentage difference (PD) between simulated and observed data is defined as

$$PD = \frac{100 \cdot (Y - X)}{X} \%$$

Where X is the observed value, and Y is the simulated value.

The standard coefficient of determination (R^2) and the Nash-Sutcliffe model efficiency (NSE) were calculated to measure goodness of fit. R^2 has been widely used, but it is oversensitive to high extreme values and insensitive to additive and proportional differences between simulated and observed data (Moriasi et al., 2007). Nash and Sutcliffe (1970) define the NSE between simulated and observed data sets as

$$NSE = 1 - \left[\frac{\sum_{i=1}^{n} \left(Y_i^{obs} - Y_i^{sim} \right)^2}{\sum_{i=1}^{n} \left(Y_i^{obs} - Y^{mean} \right)^2} \right]$$

Where Y_i^{obs} is the *i*th observed data, Y_i^{sim} is the *i*th simulated data, Y^{mean} is the mean of observed data sets, and n is the total number of observations.

A NSE value of 1.0 indicates a perfect fit of simulated and observed data. A NSE value of less than 0.0 indicates that the mean observed data is a better predictor than the simulated data, which indicates unacceptable performance (Moriasi et al., 2007).

Besides the statistical measures, graphs of various types were used to provide a visual comparison between simulated and observed flows and sediment loadings. These included time series plots of observed and simulated annual data showing PD, and scatter plots of observed versus simulated monthly data with the linear regression line and R^2 displayed.

7.5 Results and Discussion

During the 1993-2001 period, the annual precipitation in the Upper Broad Run watershed ranged from a low of 734 mm in 2007 to a high of 1359 mm in 2003, with an average of 1060 mm (Figure 7-4). The precipitation data from 1993 to 2001 were derived from PLAIN2, which was the only station available then. For the 2002-07 period, the data were area-averaged from the AIRL, RITC, and CSNY stations. Compared to the long-term average precipitation of 1016 mm from 1951 to 2007, the period from 1993 to 1997 was wetter than average, with a 1996 being a wet year. The period from 1998 to 2001 was near-average. The period from 2002 to 2007 was also near-average overall, but had the driest year being 2007 and wettest year being 2003.

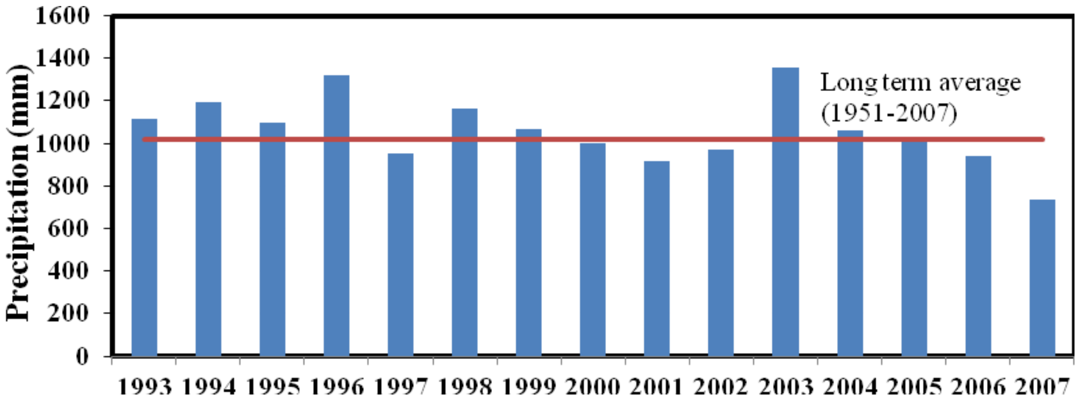


Figure 7-4: Annual Precipitation Summary from 1993 to 2007 in the Upper Broad Run Watershed

7.5.1 Flow Calibration and Prediction at Stream Station ST70

Statistical comparisons between simulated and observed flows at the stream station ST70 for Test1 and Test2 are presented in Table 7-3. Table 7-3 includes the comparisons in the three simulation periods (1993-1997, 1998-2001 and 2002-2007) representing varying climate and land use conditions, as well as the entire 15 year period from 1993 to 2007. A comparison of observed and simulated annual flows from 1993 to 2007 for Test1 and Test2 is shown in Figure 7-5. Scatter plots of observed versus simulated monthly flows for Test1 and Test2 in the three simulation periods and the entire 15 year period are given in Figure 7-6.

Model performance: Calibration

The HSPF application at the coarser segmentation in Test1 was calibrated in simulation period I from 1993 to 1997. Over the five-year calibration period for Test1, average annual flow was underestimated by 7% (Table 7-3), and the differences between annual observed and simulated flows were within 15 percent in three out of five years (Figure 7-5). The largest difference was in the wet year 1996 with an underestimation of 39%. Monthly flows during the calibration period in Test1 had a high NSE value of 0.88, indicating a good correlation, which was also reflected by the R^2 of 0.75 (Table 7-3).

The HSPF application at the finer segmentation in Test2 was calibrated in simulation period III from 2002 to 2007. Over the six-year calibration period for Test2, average annual flow was also underestimated by 7% (Table 7-3) , and there were four years with PDs between annual observed and simulated flows less than 15% (Figure 7-5). The annual flow in the wettest year 2003 was underestimated by 17%. Monthly flows during the calibration period in Test2 also had a high NSE value of 0.89 and R^2 of 0.74 (Table 7-3).

As shown in Figure 7-6, the slope of the linear regression of simulated versus observed monthly flows was less than 1.0 for both tests in their calibration periods; thus, wet period flows were generally underestimated. This could help to explain the relatively large discrepancies in the wet years of 1996 (Test1) and 2003 (Test2).

Overall, both HSPF applications in Test1 and Test2 were calibrated well for flow simulation based on monthly, annual and overall measures. Table 7-2 listed the differences of principal calibration parameters between the two tests, including LZSN (3.8 in Test1 versus 3.5 in Test2) and UZSN (0.5-0.72 in Test1 versus 0.4-0.62 in Test2). According to BASINS Technical Notes 6 (USEPA, 2000), lower zone nominal storage (LZSN) is related to both precipitation patterns and soil characteristics; whereas upper zone nominal storage (UZSN) is related to land surface characteristics, topography and LZSN. In the authors' experience, the differences in values of LZSN and UZSN between the two tests were small. The calibrations of the two tests under different precipitation patterns (test1 in wetter than average period and test2 in near average period) might help to explain the small differences. It could also be simply the result of the coarser or finer segmentation used in the two tests.

Model performance: Prediction

HSPF application in Test1

The HSPF application in Test1 was used in a predictive manner in simulation period II (1998-2001) and simulation period III (2002-2007), with metrological and land use conditions for those periods. For simulation period II, the model predicted annual flow very well in 1998 and 2001 (Figure 7-5). However, the average annual flow was over-predicted by 23% (Table 7-3) mainly because of a very large discrepancy in 1999 (+120% as shown in Figure 7-5). Compared to other years, 1999 was average with an annual precipitation of 1066 mm (Figure 7-4). However, the model predicted a very small observed annual flow in 1999, even less than the driest year 2007. There are backwater effects at station ST70, and flow is measured by an acoustic transducer. Around July 1999, the water level dropped to at or below the depth at which the transducer was installed, thus leading to inaccurate flow reading (the Accusonics transducer being used at the site requires at least a foot of water over it to read accurately). The transducer was lowered to overcome this difficulty, and flow measurements were recommenced. It is likely that the small observed flow in 1999 was due in large part to this issue. In addition, there was one thunderstorm in September recorded in the observed meteorology data, which didn't generate correspondingly high observed flow at ST70. It is possible that the thunderstorm was local to the rain gauge PLAIN2, and it did not impact the drainage area of station ST70. The PLAIN2 station is not in the Broad Run drainage basin, and there is a ridge between the station and the watershed. However, during that period, it was the closest weather station, and therefore the data from that station were used. It was in response to such issues that ten additional rain gauge sites were established in the Occoquan watershed in 2000/2001. Three of these sites are much nearer the watershed.

During simulation period III, the test1 model under-predicted average annual flow by 15% (Table 7-3). The differences between annual observed and predicted flows were within 15% in two years, and the annual flow in the wettest year 2003 was under-predicted by 26% (Figure 7-5).

As shown in Table 7-3 and Figure 7-6, the temporal variations of monthly flows were captured well during both the simulation period II and III, with high NSE values (0.85 in simulation period II and 0.86 in simulation period III) and R^2 values (0.84 in simulation II and 0.72 in simulation III).

HSPF application in Test2

The HSPF application in Test2 was used in a predictive manner in simulation period I (1993-1997) and simulation period II (1998-2001). During simulation period II, the model over-predicted average annual flow by 24% mainly because of a very large discrepancy in 1999, similar to what happened with the Test1 HSPF application, the possible reasons for which were explained above. The average annual flow was very well predicted (+2%) during the simulation period I, with over-prediction in most years and under-prediction (–31%) in the wet year 1996. As shown in Table 7-3 and Figure 7-6, the HSPF application in Test2 also captured the temporal variations of monthly flows well during both the simulation period I and II, with NSE and most R^2 values greater than 0.7.

Comparative analysis of Test1 and Test2

As expected, both the applications in Test1 and Test2 performed better in their calibration periods than in the prediction periods. The results also showed that with a good calibration under relatively long periods (5 years in Test1 and 6 years in Test2) covering different moisture regimes, the HSPF applications were able to provide robust flow predictions.

During the entire period from 1993 to 2007, both applications estimated average annual flow very well (–4% in Test1 and +2% in Test2, Table 7-3), with annual flows within 15% in seven out of fifteen years (Figure 7-5). As shown in Table 7-3 and Figure 7-6, the temporal variations of monthly flows during the entire period were captured equally well in both tests, with high NSE values (0.87 in Test1 and 0.85 in Test2) and R^2 values (0.73 in Test1 and 0.70 in Test2).

Compared to the HSPF application at the coarser segmentation in Test1, the HSPF application at the finer segmentation in Test2 didn’t show much improvement in flow simulation based on monthly, annual and long term measures. For a better flow simulation, landscape spatial variations (for example, land use distribution, slope and soil) should be accounted by an appropriate segmentation. It is likely that the coarser segmentation had accounted enough landscape spatial variations in the Upper Broad Run watershed. Therefore the finer segmentation could not improve the spatial variation accounting any more. It was found that the landscape parameters (i.e. average elevation and slope) didn't change much with the finer segmentation (Table 7-1). In addition, the differences in calibrated values of LZSN and UZSN between the two segmentations were small, as discussed earlier. These all seemed to indicate that the finer segmentation didn't provide a better accounting of landscape spatial variations.

Table 7-3: Statistical Comparisons between Observed and Simulated Flows

Indicator		Simulation period I (1993-1997)	Simulation period II (1998-2001)	Simulation period III (2002-2007)	Entire period (1993-2007)
			Average Annual		
Precipitation (cm)		113.6	103.7	101.3	106.0
Observed (10^6 m^3)		57.2	36.6	51.0	49.2
Simulated (10^6 m^3)	Test1	53.4	44.8	43.5	47.2
	Test2	58.1	45.3	47.3	50.4
Flow PD (%)	Test1	−7	23	−15	−4
	Test2	2	24	−7	2
			Monthly		
R^2	Test1	0.75	0.84	0.72	0.73
	Test2	0.69	0.73	0.74	0.70
NSE	Test1	0.88	0.85	0.86	0.87
	Test2	0.83	0.78	0.89	0.85

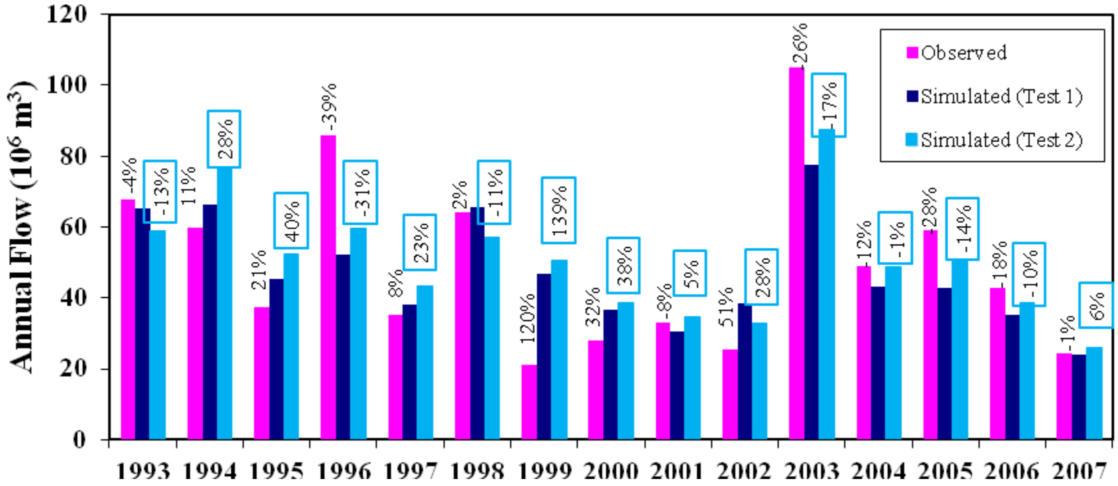


Figure 7-5: Time Series Plots of Observed and Simulated Annual Flows

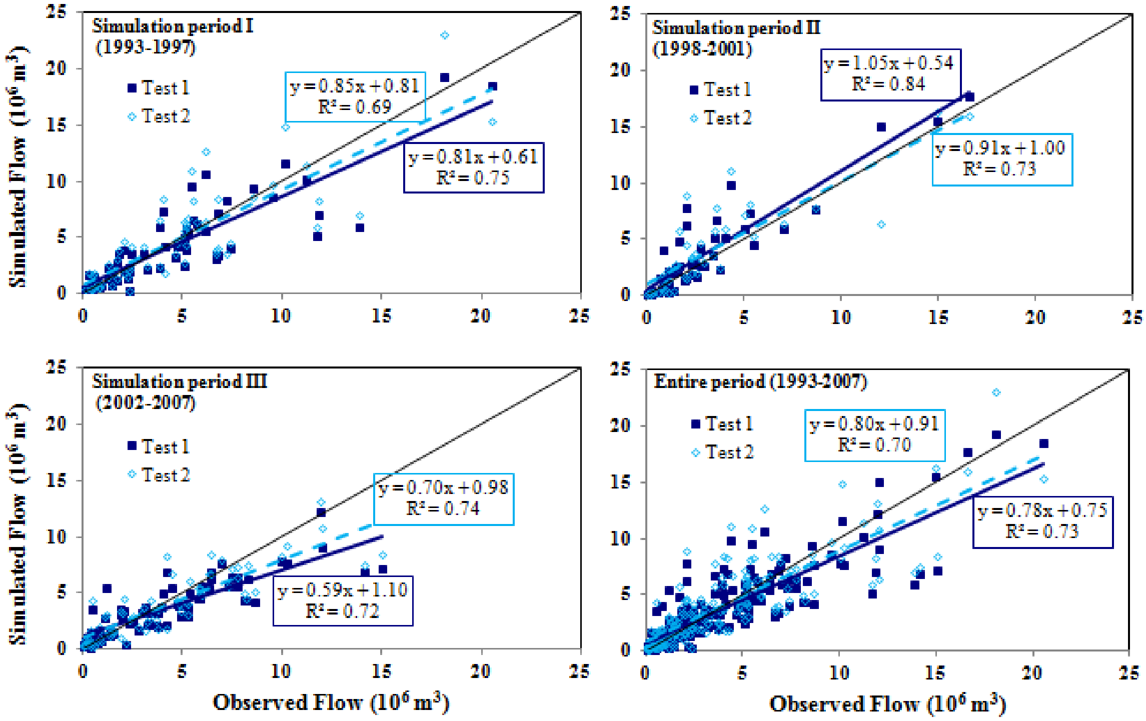


Figure 7-6: Scatter Plots of Observed and Simulated Monthly Flows

7.5.2 Sediment Calibration and Prediction at Stream Station ST70

Similar statistical and graphical measures as those that were used for the flow evaluation were applied to compare simulated and observed sediment loadings at the stream station ST70 for Test1 and Test2. Table 7-4, Figures 7-7 and 7-8 display the results of this exercise.

<u>Model performance: Calibration</u>

The HSPF application with the coarser segmentation in Test1 (1993-97) showed that, over the five-year calibration period, average annual sediment loading was underestimated by 51% (Table 7-4). The model also underestimated sediment loadings in most years, especially the wet year 1996 with a large discrepancy of 89% (Figure 7-7).

Compared to the calibration in Test1, the HSPF application with the finer segmentation in Test2 performed better in its calibration period from 2002 to 2007. Average annual sediment loading was underestimated by 21% (Table 7-4). Sediment loadings were underestimated in most years, with the underestimation magnitude being less than Test1. The annual sediment loading in the wettest year 2003 was overestimated by 24% (Figure 7-7).

The temporal variations of monthly sediment loadings were not captured well by either application in their calibration periods, with relatively low NSE values (0.32 in Test1 and 0.38 in Test2) and R^2 values (0.24 in Test1 and 0.23 in Test2). As reported in many papers (for example, USEPA, 2006; Engelmann et al., 2002; Saleh and Du, 2004), sediment is the most difficult constituent to calibrate in HSPF and requires adjusting many parameters, and yet often resulting in low NSE values.

Model performance: Prediction

When the HSPF application in Test1 was used in a predictive manner for simulation periods II and III, average annual sediment loadings were under-predicted by 72% and 24% (Table 7-4). The model under-predicted annual sediment loadings in almost all the years, especially the relatively wet year 1998. The sediment loading was over-predicted in the wettest year 2003 (Figure 7-7). The predicted monthly sediment loadings also showed weak correlations with observed values, with lower NSE values of 0.28 and –0.59 (Table 7-4). The negative NSE indicated an unacceptable model performance in the simulation period III.

The HSPF application in Test2 was better in predicting sediment loadings. Except for a large underestimation in 1998, the HSPF application in Test2 was able to predict reasonable annual sediment discharges (Figure 7-7), as well as more consistent average annual PD and monthly NSE values in the three simulation periods (Table 7-4).

Besides the better performance in the three simulation periods, the HSPF application in Test2 also simulated sediment loadings better during the entire 15 year period from 1993 to 2007, by showing a lower average annual PD (–33% versus –49%) and a higher NSE value (0.44 versus 0.16) (see Table 7-4). This result is also supported by the regression lines and R^2 values displayed in the scatter plots (Figure 7-8). The slope of the linear regression of simulated versus observed monthly sediment loadings was less than 1.0 for both tests, indicating that large sediment loadings were being under-predicted.

Overall, the HSPF application with the finer segmentation (Test2) showed noticeable improvement for sediment simulation over the coarser segmentation application (Test1). Of the principal calibration parameters in Table 7-2, each of the HSPF applications in Test1 and Test2 was quite sensitive to sediment routing parameters in reaches, including TAUCS (critical bed shear stress for scour) for silt and clay. The sediment loading simulation is greatly affected by the channel bed shear stress estimation. The accuracy of the bed shear stress estimation probably increases with a better accounting of spatial variation for channels when a finer segmentation is applied. As indicated in Table 7-1, the reach characteristics (including average reach length, slope, width and depth) represented by the finer segmentation were quite different from the coarser segmentation, indicating the possible improvement for accounting spatial variation for channels.

Table 7-4: Statistical Comparisons between Observed and Simulated Sediment Loadings

Indicator		Simulation period I (1993-1997)	Simulation period II (1998-2001)	Simulation period III (2002-2007)	Entire period (1993-2007)
		AVERAGE ANNUAL			
Observed (10^3 ton)		3.42	4.39	2.90	3.48
Simulated (10^3 ton)	Test1	1.69	1.21	2.22	1.78
	Test2	2.60	2.01	2.31	2.33
Sediment PD (%)	Test1	−51	−72	−24	−49
	Test2	−24	−54	−21	−33
		MONTHLY			
R^2	Test1	0.24	0.36	0.11	0.13
	Test2	0.33	0.56	0.23	0.33
NSE	Test1	0.32	0.28	−0.59	0.16
	Test2	0.48	0.43	0.38	0.44

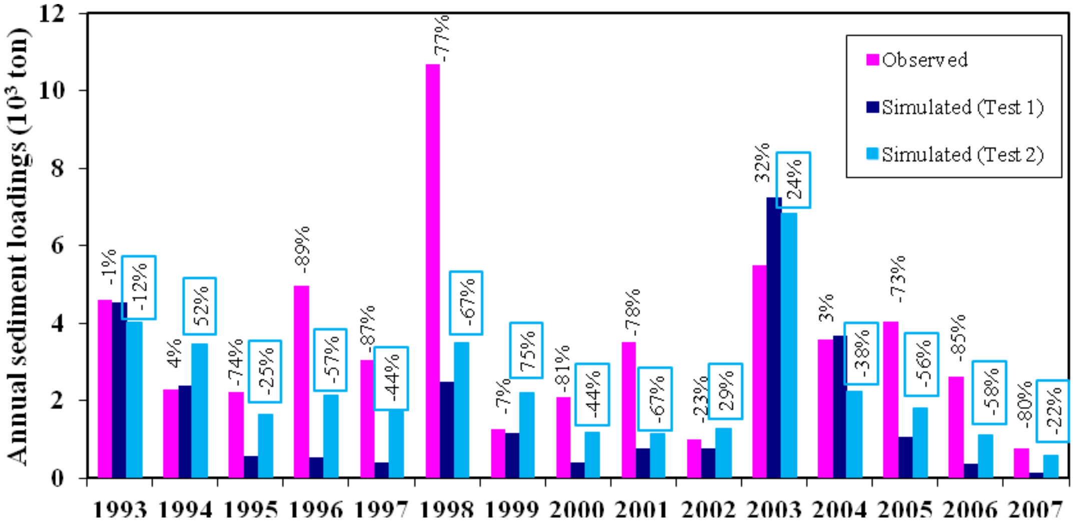


Figure 7-7: Time Series Plots of Observed and Simulated Annual Sediment Loadings

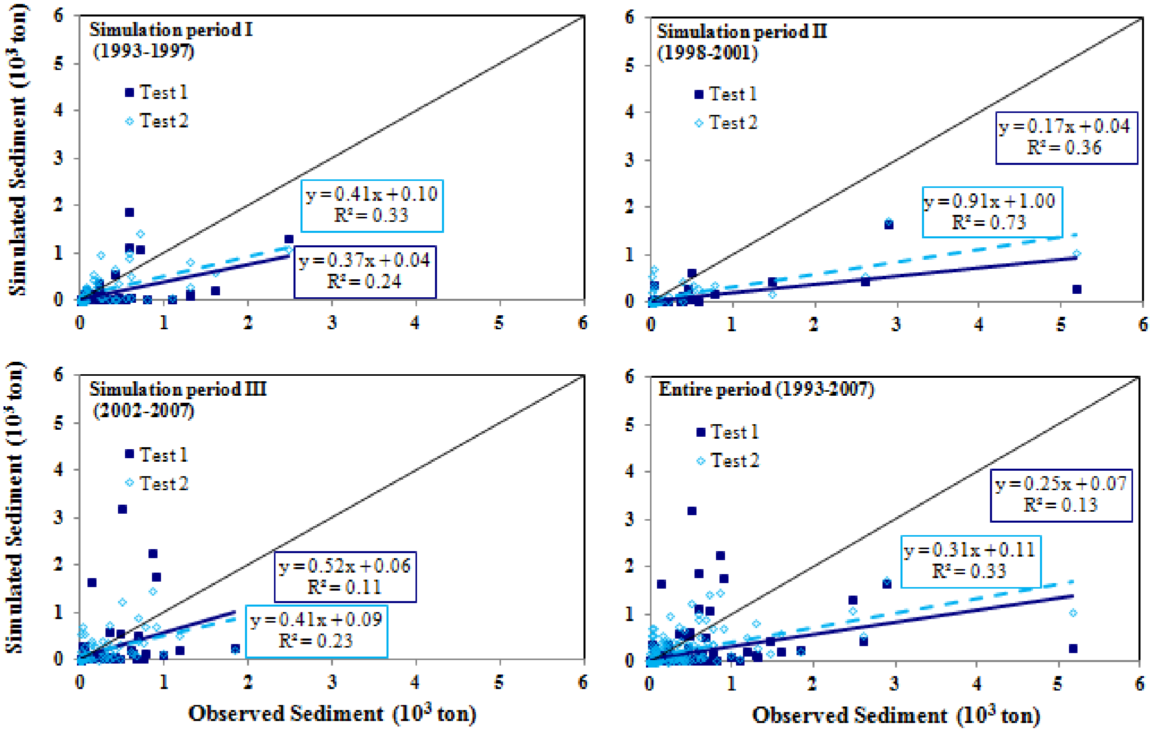


Figure 7-8: Scatter Plots of Observed and Simulated Monthly Sediment Loadings

7.6 Conclusions

Two HSPF applications for the Upper Broad Run watershed, one calibrated for 1993-97 at a coarser segmentation and one calibrated for 2002-07 at a finer segmentation, were used in a predictive manner for other periods to assess HSPF performance of flow and sediment prediction. Comparisons between observed and simulated flows and sediment loadings at the stream station ST70 were used in evaluating model performance.

Based on statistical and graphical comparisons, both applications calibrated well for flow. Flow was also predicted reasonably well when the applications were extended 10 years beyond their calibration periods with varying climate and land use conditions, indicating the robustness of flow prediction. The comparisons showed that no one application was best under all conditions. Also, the characteristics of simulated flows with both applications were generally similar to each other; for example, underestimating high flows. These results indicate that, for the calibration and prediction of flow, an increase of the segmentation does not have a major impact on the results.

As the most difficult constituent to calibrate in HSPF, sediment calibration was not as good as the flow calibration in the applications at both watershed segmentations. Both applications generally underestimated sediment loadings, indicating that appropriate judgment should be exercised when using the applications for sediment prediction. However, the HSPF application with the finer segmentation calibrated better and was better at predicting sediment loadings. The results also showed that the application at the finer segmentation was better under all conditions, including the three simulation periods representing varying climate and land use conditions, as well as the entire 15 year period. To obtain a better calibration and predictive capability for sediment, a finer segmentation appears to provide benefits. Most HSPF applications have short execution times. Therefore, there is very little penalty to running a model with finer segmentation to get better sediment results. The main effort is in the one-time initial set-up of the model input files, and increasing segmentation increases this effort.

The results of this study were limited to the Upper Broad Run watershed, which, with an area of 126.21 km^2, is a small-to-medium sized watershed. Important factors that have an impact on HSPF application results include watershed size, spatial distribution of precipitation data (that is, how close the rain gauges are to the watershed being modeled), as well as the modeler's experience. If the model application is set-up carefully, with appropriate segmentation, these results ought to hold up for larger watersheds, too.

7.7 References

Al-Abed, N.A., and Whiteley, H.R., 2002. Calibration of the Hydrological Simulation Program Fortran (HSPF) model using automatic calibration and geographical information systems. Hydrological Processes. 16, 3169-3188.

Arabi, M., Govindaraju, R.S., Hantush, M.M. ,and Engel, B.A., 2006. Role of watershed subdivision on modeling the effectiveness of best management practices with SWAT. *Journal of the American Water Resources Association*. 42(2): 513-528.

Bicknell, B.R., Imhoff, J.C., Kittle, J.L., Jobes, T.H., and Donigian, A.S, 2005. Hydrological Simulation Program -Fortran (HSPF). User’s manual for release 12.2. U.S.EPA. National Exposure Research Laboratory, Athens, GA.

Bingner, R.L., Garbrecht, J., Arnold, J.G., and Srinivasan, R., 1997. Effect of Watershed Subdivision on Simulation Runoff and Fine Sediment Yield. Transactions of the American Society of Agricultural Engineers 40(5): 1329-1335.

Borah, D.K., and Bera, M., 2003. Watershed-scale hydrologic and non-point-source pollution models: review of mathematical bases. Transactions of the ASAE Vol. 46(6): 1553-1566.

Borah, D.K., and Bera, M., 2004. Watershed-scale hydrologic and non-point-source pollution models: review of applications. Transactions of the ASAE Vol. 47(3): 789-803.

Borah, D.K., Bera, M., and Xia, R., 2004. Storm event flow and sediment simulations in agricultural watersheds using DWSM, Transactions of the ASAE, vol. 47, no. 5, pp. 1539-1559.

Brun, S. E., and Band, L. E., 2000. Simulating runoff behavior in an urbanizing watershed. Computers, Environ. and Urban Systems 24(1): 5−22.

Diaz-Ramirez, J.N., Perez-Alegria,v, and McAnally, W.H., 2008. Hydrology and Sediment Modeling Using HSPF/BASINS in a Tropical Island Watershed. Transactions of the ASABE 51(5):1555-1565.

Donigian, A. S., Bicknell, B. R., Patwardham, A. S., Linker, L. C., and Chang, C., 1994. Chesapeake Bay Program: watershed model application to calculate bay nutrient loadings. U.S. EPA-903-R-94-042, Chesapeake Bay Program Office, U.S.EPA. Annapolis, Maryland.

Donigian, A. S., Bicknell, B. R., and Imhoff, J. C., 1995. Hydrologic Simulation Program - FORTRAN. Computer Models of Watershed Hydrology, Water Resources Publications, V. P. Sirgh, ed., Highlands Ranch, CO, 395-442.

Donigian, A.S., Bicknell, B.R., Chinnaswamy, R.V., and Deliman, P.N., 1998. Refinement of a Comprehensive Watershed Water Quality Model with Application to the Chesapeake Bay Watershed. Technical Report EL-98-6. U.S. Army Corps of Engineers, Waterways Experiment Station, Vicksburg, MS. 244p.

Donigian, A. S., 2002. Watershed Model Calibration and Validation: The HSPF Experience. National TMDL Science and Policy Specialty Conference 2002, Phoenix, Arizona, Water Environment Federation.

Engelmann, C. J. K., Ward, A. D., Christy, A. D., and Bair, E. S., 2002. Application of the BASINS database and NPSM model on a small Ohio watershed. J. American Water Resources Assoc.38(1): 289−300.

FitzHugh, T. W., and MacKay, D.S., 2000. Impacts of Input Parameter Spatial Aggregation on an Agricultural Nonpoint Source Pollution Model. Journal of Hydrology 236: 35-53.

Gong, Y., Shen, A. , Liu, R., Wang, X. , and Chen, T., 2010. Effect of watershed subdivision on SWAT modeling with consideration of parameter uncertainty. Journal of Hydrologic Engineering 15(12): 1070-1074.

Hayashi, S., Murakami, S., Watanabe, M., Xu, B., 2001. HSPF simulation of runoff and sediment loads in the upper Changjiang River Basin, China. Journal of Environmental Engineering 130(7), 801–815.

Jha, M., Gassman, P.W., Secchi, S., Gu, R., and Arnold, J., 2004. Effect of Watershed Subdivision on SWAT Flow, Sediment, and Nutrient Predictions, Journal of the American Water Resources Association, 40(3), 811–825.

Laroche, A., Gallichand, J., Lagace, R., and Pesant, A., 1996. Simulating atrazine transport with HSPF in an agricultural watershed. J. Environ. Eng. 122(7): 622−630.

Mamillapalli, S., Srinivasan, R., Arnold, J.G., and Engel, B.A., 1996. Effect of Spatial Variability on Basin Scale Modeling. In: Proceedings of the Third International Conference/Workshop on Integrating GIS and Environmental Modeling. National Center for Geographic Information and Analysis, Santa Barbara, California.

Mishra, A., Kar.S, and Singh, V. P., 2007. Determination of runoff and sediment yield from a small watershed in subhumid subtropics using the HSPF model. Hydrological Processes, 21 (22): 3035-3045.

Moriasi, D.N., Arnold, J.G., Van Liew, M.W., Bingner, R.L., Harmel, R.D., Veith, T.L., 2007. Model evaluation guidelines for systematic quantification of accuracy in watershed simulations. Transactions of the ASABE. 50(3):885-900.

Nash, J.E., and Sutcliffe, J.V., 1970. River flow forcasting through conceptual models: Part 1. A discussion of principles. J. Hydrology 10 (3): 282-290.

Rahman, M., and Salbe, I., 1995. Modeling impacts of diffuse and point−source nutrients on the water quality of South Creek catchment. Environ. International 21(5): 597−603.

Saleh, A., and Du, B., 2004. Evaluation of SWAT and HSPF within BASINS Program for the Upper North Bosque river watershed in Central Texas, Transactions of the ASAE Vol. 47(4): 1039-1049.

Semmens, D., Hernandez, M., Goodrich, D.C., Kepner, W.G., 2006. A retrospective analysis of model uncertainty for forecasting hydrologic change. In: Voinov, A., Jakeman, A., Rizzoli, A. (eds). Proceedings of the iEMSs Third Biennial Meeting: "Summit on Environmental Modelling and Software". International Environmental Modelling and Software Society, July 2006, Burlington, VT.

Singh, J., Knapp, H.V., Arnold, J.G., and Demissie, M., 2005. Hydrological modeling of the Iroquois River Watershed using HSPF and SWAT. J. Am. Water Resource. Assoc. 41:343–360.

Skahill, B.E., 2004. Use of the Hydrological Simulation Program-FORTRAN (HSPF) model for watershed Studies. SMART Technical Notes Collection, ERTC/TN SMART-04-1, U.S. Army Engineer Research and Development Center, Vicksburg, MS.

United States Environmental Protection Agency (USEPA), 2000. BASINS Technical Note 6: Estimating Hydrology and Hydraulic Parameters for HSPF. EPA-823-R00-012, Washington, DC.

United States Environmental Protection Agency (USEPA), 2006. BASINS Technical Note 8: Sediment Parameter and Calibration Guidance for HSPF. Office of Water, 4305, Washington, DC.

Virginia Division of Mineral Resource (VDMR), 2001. Geology of Virginia. Available at http://www.mme.state.va.us/DMR/DOCS/Geol/vageo.html. Accessed 17 August, 2007.

Xu, Z., 2005. A complex, linked watershed-reservoir hydrology and water quality model application for the Occoquan Watershed, Virginia. PhD. Dissertation, Virginia Tech.

Xu, Z., Godrej, A.N., and Grizzard, T.J., 2007. The hydrological calibration and validation of a complexly-linked watershed-reservoir model for the Occoquan Watershed, Virginia. Journal of Hydrology, 345, 3–4: 167-183.

Chapter 8. Conclusions and Recommendations

8.1 Summary

This research was done to investigate the aspects of effective modeling of nutrient losses and nutrient management practices in the Lake Manassas watershed. The hydrology and water quality activities of the watershed have been simulated using two HSPF model applications in the Upper Broad Run and Middle Broad Run subbasins, and one CE-QUAL-W2 model application for Lake Manassas.

The HSPF software, with its AGCHEM module, provides a detailed simulation of the dynamic and continuous processes that affect the storages and outflow of nutrients from a watershed. However, extensive data requirements and complicated module setup prevent AGCHEM from being widely used. Uses of AGCHEM have not been well documented. The primary goal of this research was to investigate the AGCHEM module of HSPF for effective nutrient simulation. The goal was achieved by completing the following research objectives:

1. To investigate important inputs and parameters of HSPF/AGCHEM application for nutrient simulation in the Upper Broad Run subbasin. To effectively model nutrient losses, these inputs and parameters have to be estimated as accurate as possible. By focusing on the significant inputs and parameters, one can also expect to save time and effort involved in applying HSPF/AGCHEM.

2. To compare the AGCHEM module with PQUAL (the other simpler nutrient simulation algorithm of HSPF) in the Upper Broad Run subbasin. A significant concern is to establish if AGCHEM can provide sufficiently more accurate nutrient modeling results than PQUAL, thus making the time and effort involved in using AGCHEM worthwhile.

3. To apply HSPF/AGCHEM within a linked watershed-reservoir model system to evaluate nutrient management practice in the Lake Manassas watershed. The linked watershed-

reservoir model approach is being used for effective nutrient simulation when a watershed drains into a larger waterbody. The significant concerns are if HSPF/AGCHEM can provide a good linkage with reservoir model and if such linkage can be well-applied to evaluate nutrient management practice.

Integral to the research objectives was to develop, calibrate and validate 1) HSPF/PQUAL model application in Upper Broad Run subbasin; 2) HSPF/AGCHEM model application in Upper Broad Run subbasin; 3) HSPF/AGCHEM model application in Middle Broad Run subbasin; 4) CE-QUAL-W2 model application in Lake Manassas. These models were developed in the simulation period from 2002 to 2007, calibrated using observed data for 2002-05 (consisting of average-to-somewhat-wet years) and validated for 2006-07 (consisting of dry and average years). The main steps included:

- Performing delineation and segmentation for the Lake Manassas watershed. As a result, the watershed was simulated using 7 and 4 segments for the Upper Broad Run and Middle Broad Run subbasins, respectively. Lake Manassas was simulated using a total of 32 active computational segments, with computational layers at full pool ranging from 1 to 34, each 0.5 m thick.

- Developing the HSPF/PQUAL model for the Upper Broad Run subbasin. The 2006 land use data were consolidated into nine land use categories for this simulation: forest, pasture, high tillage cropland, low tillage cropland, townhouse/garden apartment, low density residential, medium density residential, industrial/commercial, and institutional. Precipitation data were obtained from 3 rain gauges close to the Upper Broad Run subbasin. Other meteorological data were obtained from the Washington Dulles International Airport weather station: air temperature, cloud cover, dew point temperature, potential evapotranspiration (ET), solar radiation, and wind speed. Observed data from stream station ST70 were used to calibrate the model. Hydrology was calibrated first, then sediment, and, lastly, water quality.

- Developing the HSPF/AGCHEM model for the Upper Broad Run subbasin. The flow and sediment simulation were kept same as the Upper Broad Run HSPF/PQUAL model. The PQUAL module was replaced by AGCHEM for nutrient simulation. For the AGCHEM application, the high and low tillage croplands were split into hay, high tillage corn, low tillage corn, wheat, and soybean, based on cropland distributions in Fauquier County. Nutrient inputs from atmospheric deposition, fertilization and manure application were required for the AGCHEM application. Extensive efforts were made to estimate fertilization and manure inputs. Manure was only applied for pasture, and fertilizer was applied for all other land uses except forest. Generally, one typical fertilizer application (including application rate, timing and technique) was developed separately for each fertilized land use, based on recommendations from the Virginia Nutrient Management Standards and Criteria (VDCR, 2005) and personal discussions with Fauquier county Extension agents (Ohlwiler, 2009; Marshall, 2009). The typical fertilizer application was assumed to be taken for the whole subbasin, and repeated every year over the entire simulation period. The model calibration focused on comparing simulated and observed nutrient (OP, NH_4-N, Ox-N) loadings at stream station ST70.

- Developing the HSPF/AGCHEM model for the Middle Broad Run subbasin. The required data were similar to the Upper Broad Run HSPF/AGCHEM model, including meteorological data, land use data and nutrient inputs. Precipitation data were obtained from 3 rain gauges closer to the Middle Broad Run subbasin. Cropland distributions, manure and fertilizer recommendations in Prince William County were used while developing the Middle Broad Run HSPF/AGCHEM model. Because the Middle Broad Run subbasin is ungauged, calibration parameters from the Upper Broad Run HSFP/AGCHEM model were used for the Middle Broad Run model.

- Developing the CE-QUAL-W2 model for Lake Manassas. The required data included meteorological data (air temperature, cloud cover, dew point temperature, precipitation, solar radiation, wind speed and wind direction) and boundary inputs (daily time series of upstream flow, tributary flow, distributed tributary flow, water withdrawal, and water quality associated with incoming flows). Upstream flow and associated water quality data were provided by the calibrated Upper Broad Run HSPF/AGCHEM model. The tributary and distributed tributary flows along the lake and associated water quality were provided by the Middle Broad Run HSPF/AGCHEM model. Observed data at five lake stations (LM01, LM03, LM04, LM05 and LM06) were used for the CE-QUAL-W2 model calibration, which started from the water budget calibration and was followed by heat budget calibration and water quality calibration.

8.1.1 First Objective

The first objective was to investigate important inputs and parameters of the HSPF/AGCHEM model for nutrient simulation. This was achieved by performing “one-variable-at-a-time” sensitivity analysis for the calibrated Upper Broad Run HSPF/AGCHEM model to examine the sensitivity of nutrient (NH_4-N, Ox-N, OP) loadings with respect to model inputs and parameters. Seven meteorological inputs, 4 nutrient inputs (atmospheric, manure and fertilizer application rates, and fertilizer application time) and 103 parameters related to streamflow generation, sediment and nutrient transport and interactions on lands and within streams were included in the sensitivity analysis. Sensitivity results were presented for both average yearly and average seasonal (spring, summer, fall, winter) nutrient loadings.

The sensitivity analysis leads to the following conclusions:

- Accurate meteorological inputs (especially precipitation) and hydrologic simulation are very important for effective nutrient modeling. This confirms the significance of site-specific precipitation data. In 2001, OWML established new rain gauge stations in the Occoquan watershed to provide more precipitation coverage. This effort is so worthwhile!

- Fertilizer inputs are very important for nutrient load generation. Nutrient loadings are positively correlated with the fertilizer application rate. Changing fertilizer application times has significant impacts on seasonal nutrient loadings. To effectively use the

AGCHEM module for nutrient simulation, the fertilizer inputs must be estimated as accurately as possible. By showing sensitivity to changes in fertilizer application rate and time, the flexibility of using AGCHEM for evaluating alternative nutrient management practices is demonstrated.

- The sensitive AGCHEM parameters describing nitrogen and phosphorus cycles in the soil included: NITR parameters describing ammonium adsorption and desorption in groundwater layer (for NH_4-N loading), plant uptake target of nitrogen (for Ox-N loading), PHOS parameters describing phosphorus adsorption and desorption in upper layer (for OP loading). More attention should be given to these processes and parameters when applying the AGCHEM module.

- Most sensitive inputs and parameters became a little more significant in summer, probably associated with intense storm events and higher ET (potential evapotranspiration).

- Nutrient loads are not sensitive to REACH parameters describing chemical and biological processes within streams. This is possibly related to the shallow and quick-moving nature of streams. When calibrating nutrient loadings, more attention might need to be given to the pollutant generation processes on lands than the nutrient reactions in streams.

8.1.2 Second Objective

The second objective was to compare the AGCHEM and PQUAL modules of HSPF for nutrient simulation. This was achieved by conducting a side by side comparison of the Upper Broad Run HSPF/PQUAL and HSPF/AGCHEM models. The comparison was mainly based on the model performance for simulating nutrient (NH_4-N/Ox-N/OP) loadings from the watershed and in-stream nutrient (NH_4-N/Ox-N/OP) concentrations. Model capabilities were also considered in the comparison.

Model performance for nutrient loadings

Model calibration and validation were performed by comparing simulated nutrient (NH_4-N/Ox-N/OP) loadings with observed values on annual, seasonal and monthly scales. Both PQUAL and AGCHEM provided good to reasonable predictions of nutrient (NH_4-N/Ox-N/OP) loadings during the calibration and validation periods.

AGCHEM performed better than PQUAL for predicting OP loads, especially during validation years 2006 and 2007. The PD values of annual OP loads by PQUAL were –65.2% for 2006 and –56.2% for 2007, much worse than those by AGCHEM (PD=–33.5% for 2006 and PD=–13.6% for 2007).

For NH_4-N and Ox-N, although both algorithms did equally well in simulating the annual loads, PQUAL captured temporal variations in the loads better than AGCHEM. AGCHEM predicted somewhat higher NH_4-N and Ox-N loads in spring, especially in March 2003 and May 2003. This was possibly associated with the quality of nitrogen fertilizer input data used for the AGCHEM application.

Model performance for nutrient concentrations

Both algorithms were able to predict the general trends in observed nutrient (OP, NH_4-N, Ox-N) concentrations. Simulated nutrient concentrations were similar. AGCHEM performed slightly better than PQUAL for predicting storm OP concentrations during the validation period.

Model capabilities

Use of AGCHEM successfully tracked the various components of nutrient (nitrogen and phosphorus) balance for the main fertilized land types. The primary nutrient input was PO_4, NH_4 and NO_3 application from fertilizer and manure. The primary nutrient output was by plant uptake. Compared to PO_4 and NH_4, NO_3 was easier to leach and transport with subsurface flow. In addition, hay, high and low tillage corn, and wheat land uses seemed to contribute more of the nutrient loadings from the watershed.

Based on “one-variable-at-time” sensitivity analysis for the HSPF/PQUAL model in the Upper Broad Run subbasin, the OP and NH_4-N loads were sensitive to PQUAL parameters describing pollutant buildup and washoff at land surface, and the sensitive parameter for Ox-N load was groundwater nitrate concentration. These parameters are mainly determined by model calibration, and there are no direct connections of these parameters to physical characters. Therefore, PQUAL may not provide the level of detail and the capabilities needed to simulate nutrient management practices.

With accurate inputs and parameters, AGCHEM can provide sufficiently more accurate nutrient modeling results than PQUAL. However, good quality data on the extensive inputs and parameters required by AGCHEM might not be available, which could impact the model performance significantly. Whether one will choose AGCHEM depends on the data availability, required modeling accuracy, the modeler’s time and experience, and model purpose. As more TMDL studies are being performed, the use of models for management planning and alternatives analysis is increasing. Compared to PQUAL, AGCHEM has an advantage for TMDL studies that have a complex nutrient component.

8.1.3 Third Objective

The third objective was to apply HSPF/AGCHEM within a linked watershed-reservoir model system to evaluate nutrient management practices. This was achieved by 1) developing, calibrating and validating the linked watershed-reservoir model in the Lake Manassas watershed, consisting of two HSPF/AGCHEM models and one CE-QUAL-W2 model; and, 2) conducting a pre-BMP scenario analysis.

1) Water surface elevation (WSE) at the Lake Manassas dam was very well reproduced by the Lake Manassas CE-QUAl-W2 model, indicated by high R^2 values of 0.987 and 0.958 in the

calibration and validation periods. The CE-QUAL-W2 model captured the seasonal patterns for temperature and DO concentrations well, and successfully captured summer stratification in the lake.

The calibration and validation results at five lake stations (LM01, LM03, LM04, LM05 and LM06) indicated that the CE-QUAL-W2 model captured spatial trends of nutrient (OP, NH_4-N and Ox-N) concentrations at both surface and bottom layers fairly well. The model reproduces the temporal distribution of NH_4-N and Ox-N concentrations very well. Both timing and magnitude of the seasonal nitrogen cycle at surface and bottom layers were well simulated. CE-QUAL-W2 captured the OP seasonal trends in the lake fairly well. Although the model under-predicted some high bottom OP concentrations, the timing of bottom OP release was generally captured. The CE-QUAL-W2 model also reproduced algae blooms well during the summers, by showing a fair match between simulated and observed surface chl *a* concentrations at LM01.

By using the generated flow and pollutant loadings from the Upper Broad Run and Middle Broad Run HSPF/AGCHEM models, the CE-QUAL-W2 model was adequately calibrated/validated to reproduce water budget, thermal stratification, and algae/nutrient/DO dynamics in the Lake Manassas. This indicates that the HSPF/AGCHEM model can provide a good linkages with the CE-QUAL-W2 model.

2) The calibrated watershed-reservoir model was used to investigate water quality impacts by implementing nutrient management plan in the watershed. For the evaluation, a pre-BMP scenario was designed to compare with the current simulation. In the current simulation, N and P fertilizer applications were based on the recommendations of Virginia Cooperative Extension considering the nutrient management plan. The pre-BMP scenario reflected N and P fertilizer application rate changes in the past 20 years, which were estimated to be 110% of the current N fertilizer and 175% of the current P fertilizer.

The pre-BMP scenario analysis results confirmed that without the nutrient management plan, OP loads would have increased. If the pre-BMP fertilizer application rate was used, the average annual OP load from the Upper Broad Run subbasin would be much higher (about 179.6% of the current load). Under the pre-BMP scenario, the OP yield increased more in agricultural intensive areas. Therefore, implementing nutrient management plan is particularly helpful to reduce NPS in agriculturally dominated watersheds. For urban dominated watersheds, other BMPs might be better solutions to control NPS.

Without the nutrient management plan, the increase of external OP loads would have lead to accumulation of OP in the Lake Manassas. If the pre-BMP fertilizer application rate was used, higher OP concentrations would be found at both surface and bottom layers in the lake. The higher OP concentrations would have stimulated algae growth and worsen the water quality issues. It appears that implementing the nutrient management plan in the Lake Manassas watershed played an important role in reducing the nutrient enrichment and eutrophication condition of the lake.

8.2 Recommendations

The Lake Manassas watershed is a part of the larger Occoquan watershed, and, hence, a part of an Occoquan Model project. The Occoquan Model project aims to continuously improve modeling of the Occoquan watershed. Findings from this research are expected to be helpful for that project. In addition, there are several aspects that need to be further investigated with regard to the AGCHEM application and sensitivity analysis.

- In this research, the typical fertilizer application was assumed to be taken for the whole watershed, and repeated every year over the entire simulation period. Although this assumption was made based on best professional judgment, it may not accurately represent site-specific practices. A more complicated nutrient input method “special action block” in HSPF might be able to address this issue. The special action block is a generic HSPF module that allows the user to specify a particular procedure, and it can be use to allow for the nutrient input to be changed at a specified time to simulate human activities.

- HSPF/AGCHEM might be applied to other subbasins in the Occoquan watershed, especially in the agricultural-intensive Cedar Run subbasin. Nutrient loads in the Cedar Run subbasin have not been as well predicted in the Occoquan Model. In addition, the Cedar Run subbasin is larger than the Upper Broad Run subbasin and has different soil conditions. It will be even more valuable if the procedures and findings in this research can be validated in a larger watershed .

- The sensitivity analysis in this research suggests some important inputs and parameters. To effectively model nutrient losses, these inputs and parameters have to be estimated accurately. It is important to further investigate how to best estimate the important inputs and parameters.

- "One-variable-at-a-time" sensitivity analysis might be performed for other submodels in the Occoquan Model to see if the sensitive inputs and parameters vary with locations. Because other subbasins have different climate and watershed conditions, this might generate different findings.

- There are some limitations to using the "one-variable-at-a-time" sensitivity analysis, including: 1) lack of consideration of correlations between parameters; and, 2) lack of consideration of different degrees of uncertainty associated with each parameter. Future research needs to investigate other sensitivity analysis techniques to gain better insights.

- Sensitivity analysis can provide useful information for model uncertainty analysis. A complete uncertainty analysis can then help in overcome the limitations of using "one-variable-at-a-time" sensitivity analysis.

- In the long term, performing sensitivity analysis and uncertainty analysis for the linked watershed-reservoir model system might be of interest.

References Cited

Adams, B. V.,1998. Parameter Distributions for Uncertainty Propagation in Water Quality Modeling. PhD. Dissertation, Duke University.

Al-Abed, N.A., and Whiteley, H.R., 2002. Calibration of the Hydrological Simulation Program Fortran (HSPF) model using automatic calibration and geographical information systems. Hydrological Processes. 16, 3169-3188.

Arabi, M., Govindaraju, R.S., Hantush, M.M. ,and Engel, B.A., 2006. Role of watershed subdivision on modeling the effectiveness of best management practices with SWAT. *Journal of the American Water Resources Association*. 42(2): 513-528.

Baginska, B., Milne-Home, W., and Cornish, P.S., 2003. Modeling nutrient transport in Currency Creek, NSW with AnnAGNPS and PEST. Environ. Model. Software. 2003, 18, 801-808.

Beasley, D. B., Huggins, L.F., and Monke, E.J.,1980. ANSWERS: A Model for Watershed Planning. Transactions of the ASAE, 23(4), 938-944.

Bergman, M.J., Green, W., and Donnangelo, L.J., 2002. Calibration of storm loads in the south Prong watershed, Florida, using BASINS/HSPF. Journal of the American water resources association. 38(5): 1423-1236.

Bicknell, B.R., Donigian, A.S., and Barnell, T.A.,1984. Modeling Water Quality and the Effects of Agricultural Best Management Practices in the Iowa River Basin. Journal of Water Science and Technology. 17: 1141-1153.

Bicknell, B.R., Imhoff, J.C., Kittle, J.L., Jobes, T.H., and Donigian, A.S, 2005. Hydrological Simulation Program -Fortran (HSPF). User’s manual for release 12.2. U.S.EPA. National Exposure Research Laboratory, Athens, GA.

Bingner, R.L., Garbrecht, J., Arnold, J.G., and Srinivasan, R., 1997. Effect of Watershed Subdivision on Simulation Runoff and Fine Sediment Yield. Transactions of the American Society of Agricultural Engineers 40(5): 1329-1335.

Bingner, R. L., and Theurer. F. D., 2001. AnnAGNPS Technical Processes: Documentation Version 2. Available at www.sedlab.olemiss.edu/AGNPS.html. Accessed 26 July, 2010.

Borah, D.K., 2002. Watershed Scale Nonpoint Source Pollution Models: Mathematical bases. 2002 ASAE International Meeting/CIGR World Congress, Chicago, IL. Paper no. 022091.

Borah, D. K., and Bera, M., 2003. Watershed-scale hydrologic and nonpoint-source pollution models: Review of mathematical bases. Trans. ASAE 46(6): 1553-1566.

Borah, D. K., and Bera, M., 2004. Watershed-scale hydrologic and nonpoint-source pollution models: Review of applications. Trans. ASAE 47(3): 789-803.

Borah, D.K., Bera, M., and Xia, R., 2004. Storm event flow and sediment simulations in agricultural watersheds using DWSM, Transactions of the ASAE, vol. 47, no. 5, pp. 1539-1559.

Borah, D.K., Yagow, G., Saleh, A., Barnes, P.L. , Rosenthal, W., Krug, E.C., and Hauck, L.M., 2006. Sediment and nutrient modeling for TMDL development and implementation. *Transactions of the ASABE*, 49 (4): 967-986.

Bouraoui, F., and Dillaha, T. A.,1996. ANSWERS-2000: Runoff and sediment transport model. J. Environ. Eng. 122(6):493-502.

Bouraoui, F., and Dillaha, T. A., 2000. Answers-2000: Nonpoint source nutrient planning model. J. Environ. Eng. 126: 1045-1055.

Bouraoui, F., Braud, I., and Dillaha, T. A., 2002. ANSWERS: A nonpoint-source pollution model for water, sediment, and nutrient losses. Chapter 22 in Mathematical Models of Small Watershed Hydrology and Applications, 833-882.

Brown, L. C., and Barnwell, T. O., 1987. The Enhanced Stream Water Quality Models QUAL2E and QUAL2E-UNCAS: Documentation and User Manual. Environmental Resources Laboratory, Environmental Protection Agency, Athens, Georgia.

Brun, S. E., and Band, L. E., 2000. Simulating runoff behavior in an urbanizing watershed. Computers, Environ. and Urban Systems 24(1): 5−22.

Burgholzer, R., 2007. Report of a Workshop on Understanding Fertilizer Sales and Reporting Information. U.S. EPA Chesapeake Bay Program Scientific and Technical Advisory Committee and the Agricultural Nutrient Reduction Workgroup. U.S. EPA, Washington, DC.

Cerco, C.F., Linker, L., Sweeney, J., Shenk, G., and Butt, A.J., 2002. Nutrient and Solid Controls in Virginia’s Chesapeake Bay Tributaries. Journal of Water Resources Planning and Management, 128(3): 179-189.

Chesapeake Bay Program Office (CBPO), 2004. Tributary Strategy Tool. Available at http://www.chesapeakebay.net/tribtools.htm. Accessed 30 July, 2007.

Chun, K.C., Chang, R.W., Williams, G.P., Chang, Y.S., Tomasko, D., LaGoory, K., Ditmars, J., Chun, H.D., and Lee, B.K., 2001. Water quality issues in the Nakdong River basin in the Republic of Korea. Environmental Engineering and Policy. 2(3): 131-143.

Cole, T. M., and Wells, S. A., 2008. CE-QUAL-W2: A Two-Dimensional, Laterally Averaged, Hydrodynamic and Water Quality Model, Version 3.6 User Manual. In. Washington, DC: U.S. Army Corps of Engineers.

Debele, B., Srinivasan R., and Parlange. J. Y., 2006. Coupling upland watershed and downstream waterbody hydrodynamic and water quality models (SWAT and CE-QUAL-W2) for better water resources management in complex river basins. Environ Model Assess.

DePinto, J.V., Freedman, P.L., Dilks, D.M., and Larson, W.M., 2004. Models Quantify the Total Maximum Daily Load Process. Journal of Environmental Engineering, 130(6), 703-713.

Diaz-Ramirez, J.N., Perez-Alegria,v, and McAnally, W.H., 2008. Hydrology and Sediment Modeling Using HSPF/BASINS in a Tropical Island Watershed. Transactions of the ASABE 51(5):1555-1565.

Donigian, A.S., Imhoff, J.C., Bicknell, B.R., and Kittle, J.L., 1984. Application Guide for Hydrological Simulation Program - Fortran (HSPF). U.S. EPA-600/3-84-065, Environmental Research Laboratory, Athens, GA.

Donigian, A. S., Bicknell, B. R., Patwardham, A. S., Linker, L. C., and Chang, C., 1994. Chesapeake Bay Program: watershed model application to calculate bay nutrient loadings. U.S. EPA-903-R-94-042, Chesapeake Bay Program Office. U.S.EPA. Annapolis, Maryland.

Donigian, A. S., Bicknell, B. R., and Imhoff, J. C., 1995. Hydrologic Simulation Program - FORTRAN. Computer Models of Watershed Hydrology, Water Resources Publications, V. P. Sirgh, ed., Highlands Ranch, CO, 395-442.

Donigian, A.S., Bicknell, B.R., Chinnaswamy, R.V., and Deliman, P.N., 1998. Refinement of a Comprehensive Watershed Water Quality Model with Application to the Chesapeake Bay Watershed. Technical Report EL-98-6. U.S. Army Corps of Engineers, Waterways Experiment Station, Vicksburg, MS. 244p.

Donigian, A. S., Imhoff, J.C., and Kittle, J.L., 1999. HSPFParm, An Interactive Database of HSPF Model Parameters. Version 1.0. EPA-823-R-99-004. Prepared for U. S. EPA, Office of Science and Technology, Washington, D. C.

Donigian, A. S., 2002. Watershed Model Calibration and Validation: The HSPF Experience. National TMDL Science and Policy Specialty Conference 2002, Phoenix, Arizona, Water Environment Federation.

Donigian, A.S., and Love, J.T., 2007. The Housatonic River Watershed Model: Model Application and Sensitivity/Uncertainty Analysis. 7th International IWA Symposium on System Analysis and Integrated Assessment in Water Management, May 7-9, 2007. Washington, DC.

Eggink, J., 2001. An Exploration of the Limnological Dynamics of Lake Manassas. Master’s Thesis, Virginia Polytechnic Institute and State University, Falls Church, Virginia.

El-Kaddah, D.N., and Carey, A.E., 2004. Water quality modeling of the Cahaba River, Alabama. Environmental Geology. 45: 323-338.

Engelmann, C. J. K., Ward, A. D., Christy, A. D., and Bair, E. S., 2002. Application of the BASINS database and NPSM model on a small Ohio watershed. J. American Water Resources Assoc.38(1): 289−300.

Filoso, S., Vallino, J., Hopkinson, C., Rastetter, E., and Claessens, L., 2004. Modeling Nitrogen Transport in the Ipswich River Basin, Massachusetts, using a Hydrological Simulation Program Fortran (HSPF). Journal of the American Water Resources Association 40 (5): 1365–1384.

FitzHugh, T. W., and MacKay, D.S., 2000. Impacts of Input Parameter Spatial Aggregation on an Agricultural Nonpoint Source Pollution Model. Journal of Hydrology 236: 35-53.

Flowers, J. D., Hauck, L. M., and Kiesling, R., 2001. USDA: Lake Waco-Bosque River Initiative: Water Quality Modeling of Lake Waco Using CE-QUAL-W2 for Assessment of Phosphorus Control Strategies. Texas.

Fontaine, T. A., and Jacomino, V. M. F, 1997. Sensitivity analysis of simulated contaminated sediment transport. JAWRA 33: 313-326.

Gao, Q., Zhang, X., Huang, Y., and Xu, H., 2004. A comparative analysis of four models of photosynthesis for 11 plant species in the Loess Plateau. Agricultural and Forest Meteorology 126: 203–222.

Gatling, L. A., Kardash, A. O., and Yoon, J., 2000. Spatiotemporal Water Quality Modeling of Pipeline Water Intake Lake Gaston, Virginia. Paper presented at the Building Partnerships - 2000 Joint Conference on Water Resource Engineering and Water Resources Planning and Management, Virginia.

Gong, Y., Shen, A. , Liu, R., Wang, X. , and Chen, T., 2010. Effect of watershed subdivision on SWAT modeling with consideration of parameter uncertainty. Journal of Hydrologic Engineering 15(12): 1070-1074.

Gorrie, J.R., 2007. An Examination Of Water Quality Impacts On Lake Manassas. Master Thesis, Virginia Polytechnic Institute and State University, Falls Church, Virginia.

Griensven, A.V., Meixner, T., Grunwald, S., Bishop, T., Diluzio, M., and Srinivasan, R., 2006. A global sensitivity analysis tool for the parameters of multi-variable catchment models. Journal of Hydrology, 324: 10–23.

Hantzche, N. N., and Finnemore, E.J., 1991. Predicting ground-water nitrate-nitrogen impacts. Groundwater, 30 (4): 490-499.

Hayashi, S., Murakami, S., Watanabe, M., and Xu, B., 2001. HSPF simulation of runoff and sediment loads in the upper Changjiang River Basin, China. Journal of Environmental Engineering 130(7), 801–815.

Huber, W. C., and Dickinson, R. E.,1988. Storm Water Management Model User's Manual, Version 4. Athens, Georgia, Environmental Protection Agency.

Im, S., Brannan, K.M., and Mostaghimi, S., 2003. Simulating Hydrology and Water Quality Impacts in an Urbanizing Watershed. JAWRA 39(6): 1465-1479.

Imhoff, J.C., Kittle, J.L., Gonzales, B.B., Donigian, A.S., Deliman, P.N., Elliot, W.J., and Flanagan, D.C., 2010. Development and Demonstration of a Hybrid Modeling Capability within the Fort Benning HSPF Watershed Model: Refinement of Unpaved Road Simulation Using WEPP:Road. Proceedings of AWRA 2010 Spring Specialty Conference. March 29-31, 2010. Orlando, FL.

Jha, M., Gassman, P.W., Secchi, S., Gu, R., and Arnold, J., 2004. Effect of Watershed Subdivision on SWAT Flow, Sediment, and Nutrient Predictions, Journal of the American Water Resources Association, 40(3), 811–825.

Johnston, C.A., Grizzard, T.J., Godrej, A.N, and Post, H., 2000. Comparison of Two Tributary Pollutant Loading Rate Calculation Methods Using Continuous and Discrete Monitoring Data. Unpublished.

Kieffer, J.M., 2002. Development of a nutrient and dissolved oxygen water quality model for the Saint Louis Bay watershed. M.S. thesis, Mississippi State University.

Laroche, A., Gallichand, J., Lagace, R., and Pesant, A., 1996. Simulating atrazine transport with HSPF in an agricultural watershed. J. Environ. Eng. 122(7): 622−630.

Lence, B. J., and Takyi, A. K.,1992. Data Requirements for seasonal discharge programs: An Application of a Regionalized Sensitivity Analysis. Water Resources Research. 28 (7): 1781-1789.

Lenhart, T., Eckhardt, K., Fohrer, N., and Frede, H. G., 2002. Comparison of two different approaches of sensitivity analysis. Phys. Chem. Earth, 27(9-10), 645-654.

Liu, Z., 2006. Effective Modeling of Agricultural Practices within Large-scale Hydrologic and Water Quality Simulations. PhD. Dissertation, Mississippi State University.

Liu, Z., Kieffer, J. M., Hashim, N.B., Kingery, W.L., and Huddleston, D.H., 2005. The Influence of Crop Fertilization Practices on Nutrient Input Parameters for Water Quality Modeling in the Wolf River Watershed Using HSPF. International Journal of Civil and Environmental Engineering. 1(1): 1-17.

Liu, Z., Kingery, W.L., Huddleston, D. H., Hossain, F., Hashim N. B., and Kieffer J. M., 2008. Application and evaluation of two nutrient algorithms of Hydrological Simulation Program Fortran in Wolf River watershed. Journal of Environmental Science and Health, Part A 43(7):738-48.

Liu, Y., Godrej, A.N., and Grizzard, T.J., 2011a. Sensitivity Analysis, Calibration and Validation of a Watershed Model Application using HSPF with the Nutrient Algorithm PQUAL in Upper Broad Run Watershed, VA. In Submission.

Liu, Y., Godrej, A.N., Grizzard, T.J., and Dillaha, T. A., 2011b. Application and Sensitivity Analysis of a Watershed Model Application using HSPF with the Nutrient Algorithm AGCHEM in Upper Broad Run Watershed, Virginia. In Submission.

Mamillapalli, S., Srinivasan, R., Arnold, J.G., and Engel, B.A., 1996. Effect of Spatial Variability on Basin Scale Modeling. In: Proceedings of the Third International Conference/Workshop on Integrating GIS and Environmental Modeling. National Center for Geographic Information and Analysis, Santa Barbara, California.

Marshall, J., 2009. Personal Communication. Fauquier County Soil and Water Conservation District, Virginia.

Mishra, A., Kar.S, and Singh, V. P., 2007. Determination of runoff and sediment yield from a small watershed in subhumid subtropics using the HSPF model. Hydrological Processes, 21 (22): 3035-3045.

Moore, L.W., Matheny, H., Tyree, T., Sabatini, D., and Klaine, J., 1988. Agricultural Runoff Modeling in a Small West Tennessee Watershed, Journal Water Pollution Control Federation. 60(2): 242-249.

Moriasi, D.N., Arnold, J.G., Van Liew, M.W., Bingner, R.L., Harmel, R.D., Veith, T.L., 2007. Model evaluation guidelines for systematic quantification of accuracy in watershed simulations. Transactions of the ASABE. 50(3):885-900.

Mostaghimi, S., Park, S. W., Cooke, R.A, and Wang S.Y., 1997. Assessment of Management Alternatives on a Small Agricultural Watershed. Water Research 31(8): 1867-1878.

Nash, J.E., and Sutcliffe, J.V., 1970. River flow forcasting through conceptual models: Part 1. A discussion of principles. J. Hydrology 10 (3): 282-290.

Nasr, A., Bruen, M., Jordan, P., Kiely, G., Moles, R., and Byrne, P., 2007. A comparison of SWAT, HSPF and SHETRAN/GOPC for modeling phosphorus export from three catchments in Ireland. Water Research 41: 1065-1073.

Neitsch, S.L., Arnold, J.R., Kiniry, J.R., Williams, J.R., and King, W.K., 2002. Soil and Water Assessment Tool Theoretical Documentation Version 2000. Texas Water Resources Institute, College Station, Texas.

Northern Virginia Planning District Commission (NVPDC). 1994. Mission Statement for the Occoquan Basin Model Upgrade. Annandale, Virginia: Northern Virginia Planning District Commission.

Ohlwiler, T., 2009. Personal Communication. Fauquier County Cooperative Extension Office, Virginia.

Rahman, M., and Salbe, I., 1995. Modeling impacts of diffuse and point source nutrients on the water quality of South Creek catchment. Environment International. 21(5): 597-603.

Ravalico, J.K., Maier, H.R., Danday, G.C., Norton, J.P. , and Croke, B.F.W., 2005. A comparison of sensitivity analysis techniques for complex models for environment management. Proceedings of the International Congress on Modelling and Simulation, 2005/A. Zerger and R. M. Argent.

Saleh, A., and Du, B., 2004. Evaluation of SWAT and HSPF within BASINS Program for the Upper North Bosque river watershed in Central Texas. Transactions of the ASAE Vol. 47(4): 1039-1049.

Santhi, C., Arnold, J. G., Williams, J. R., Dugas, W. A., Srinivasan, R., and Hauck, L. M., 2001. Validation of the SWAT model on a large river basin with point and nonpoint sources. J. American Water Resources Assoc. 37(5): 1169−1188.

Semmens, D., Hernandez, M., Goodrich, D.C., Kepner, W.G., 2006. A retrospective analysis of model uncertainty for forecasting hydrologic change. In: Voinov, A., Jakeman, A., Rizzoli, A. (eds). Proceedings of the iEMSs Third Biennial Meeting: "Summit on Environmental Modelling and Software". International Environmental Modelling and Software Society, July 2006, Burlington, VT.

Shoemaker, C. A., and Benaman, J., 2003. A Methodology for Sensitivity Analysis in Complex Distributed Watershed Models. Philadelphia, PA, United States.

Shoemaker, L., Dai, T., Koenig, J., and Hantush, M., 2005. TMDL model evaluation and research needs. EPA/600/R-05/149.Cincinnati, Ohio: U.S. EPA, National Risk Management Research Laboratory.

Singh, J., Knapp, H.V., Arnold, J.G., and Demissie, M., 2005. Hydrological modeling of the Iroquois River Watershed using HSPF and SWAT. J. Am. Water Resource. Assoc. 41:343–360.

Skahill, B.E., 2004. Use of the Hydrological Simulation Program-FORTRAN (HSPF) model for watershed Studies. SMART Technical Notes Collection, ERTC/TN SMART-04-1, U.S. Army Engineer Research and Development Center, Vicksburg, MS.

Skinner, R.H., Corson, M.S., and Rotz, C.A., 2008. Comparison of Two Pasture Growth Models of Differing Complexity. Agricultural Systems 99: 35-43.

Suttles, J.B., Vellidis, G., Bosch, D., Lowrance, R., Sheridan, J.M., Usery, E.L., 2003. Watershed-scale simulation of sediment and nutrient loads in Georgia Coastal Plain streams using the Annualized AGNPS model. Trans. ASAE 2003, 46, 1325-1335.

Tang, Y., Reed, P., Wagener, T., and Van Werkhoven, K., 2007. Comparing sensitivity analysis methods to advance lumped watershed model identification and evaluation. Hydrology. Earth Syst. Sci., 11, 793-817.

Tsihrintzis, V.A., Fuentes, H.R., and Gadipudi, R.K., 1996. Modeling prevention alternatives for nonpoint source pollution at a Wellfield in Florida. American Resources Bulletin. 32(2): 317-331.

United States Department of Agriculture (USDA), 1992. Agricultural Waste Management Field Handbook. Natural Resources Conservation Service, Washington, DC

U.S. Department of Agriculture (USDA), 2004. National Agricultural Statistics Service. 2002 census of agriculture. Available at http://www.nass.usda.gov/census.

United States Environmental Protection Agency (USEPA), 1999. Protocal for developing nutrient TMDLs. EPA 841-B-99-007. Office of Water, Washington, DC.

United States Environmental Protection Agency (USEPA), 2000. BASINS Technical Note 6: Estimating Hydrology and Hydraulic Parameters for HSPF. EPA-823-R00-012, Washington, DC.

United States Environmental Protection Agency (USEPA), 2002. National Water Quality Inventory 2000 Report. EPA-841-R-02-001, Washington, DC.

U.S. Environmental Protection Agency (USEPA), 2004. Users Manual for AQUATOX (Release 2): Modeling Environmental Fate and Ecological Effects in Aquatic Ecosystems Volume 1. EPA-823-B-04-001. Washington, D.C.: U.S. Environmental Protection Agency, Office of Water.

United States Environmental Protection Agency (USEPA), 2006. BASINS Technical Note 8: Sediment Parameter and Calibration Guidance for HSPF. Office of Water, 4305, Washington, DC.

U.S. Natural Resources Conservation Service (NRCS), 2006. National Conservation Practice Standard: Nutrient Management. Code 590, Fort Worth, TX.

Vache, K. B., Eilers, J. M., and Santelmann, M. V., 2002. Water quality modeling of alternative agricultural scenarios in the U.S. corn belt. J. American Water Resources Assoc. 38(3): 773−787.

Virginia Division of Mineral Resource (VDMR), 2001. Geology of Virginia. Available at http://www.mme.state.va.us/DMR/DOCS/Geol/vageo.html. Accessed 17 August, 2007.
Virginia Department of Conservation and Recreation (VDCR), 2005. Virginia Nutrient Management Standards and Criteria.

Walker, W. W., 1986. Empirical Methods for Predicting Eutrophication in Impoundments; Report 3, Phase III: Applications Manual. Technical Report E-81-9. Vicksburg, Miss.: U.S. Army Engineers Waterways Experiment Station.

Wetzel, R.G., 2001. Limnology: Lake and River Ecosystems, Third Edition. Academic Press, San Diego, California.

White, K. L., and Chaubey, I., 2005. Sensitivity Analysis, Calibration, and Validations for a Multisite and Multivariable SWAT Model. Journal of American Water Resources Association 41(5):1077-1089.

Wool, T. A., Ambrose, R. B., Martin, J. L., and Cormer, E. A., 2003. Water Quality Analysis Simulation Program (WASP) Version 6.0 Draft: User's Manual. In. Atlanta, Georgia: U.S. Environmental Protection Agency.

Wu, J., 2004. Water-quality-based BMP design approach and uncertainty analysis for integrated watershed management. PhD. Dissertation, University of Virginia.

Xu, Z., 2005. A complex, linked watershed-reservoir hydrology and water quality model application for the Occoquan Watershed, Virginia. PhD. Dissertation, Virginia Tech

Xu, Z., Godrej, A.N., and Grizzard, T.J., 2007. The hydrological calibration and validation of a complexly-linked watershed-reservoir model for the Occoquan Watershed, Virginia. Journal of Hydrology, 345, 3–4: 167-183.

Young, R.A., Onstad, C.A., Bosch, D.D., and Anderson, W.P., 1994. Agricultural Non-Point Source Pollution Model, Version 4.03 AGNPS User’s Guide. U.S. Department of Agriculture, Washington, D.C.

Yuan, Y., Mehaffey, M. H., Lopez, R. D., Bingner, R. L., Bruins, R. J., Erickson, C. L., and Jackson, M., 2011. AnnAGNPS Model Application for Nitrogen Loading Assessment for the Future Midwest Landscape Study. JOURNAL OF WATER SRT - AQUA. Blackwell Publishing, Malden, MA, 3(1):196-216.

Zheng Y., and Keller, A. A., 2006. Understanding parameter sensitivity and its management implications in watershed-scale water quality modeling. Water Resource. Res., 42, W05402.

Appendix. Nutrient Inputs for HSPF/AGCHEM Applications in Lake Manassas Watershed, Virginia

The watershed model HSPF with nutrient algorithm AGCHEM was used for simulating nutrient transport and fate in the Lake Manassas watershed. The watershed was simulated using two HSPF/AGCHEM models in the Upper Broad Run and Middle Broad Run subbasins. This document describes the development of nutrient inputs for the AGCHEM applications in detail.

Description of AGCHEM

The AGCHEM module applies a nutrient balance approach as the foundation for simulating complex nutrient processes in the soil explicitly. Figure 1 shows the soil nutrient storage, nutrient application and subsequent nutrient movement and transformation in the soil profile simulated by AGCHEM. The soil profile is divided into four layers, including surface, upper, lower and groundwater, for moisture and nutrient storage.

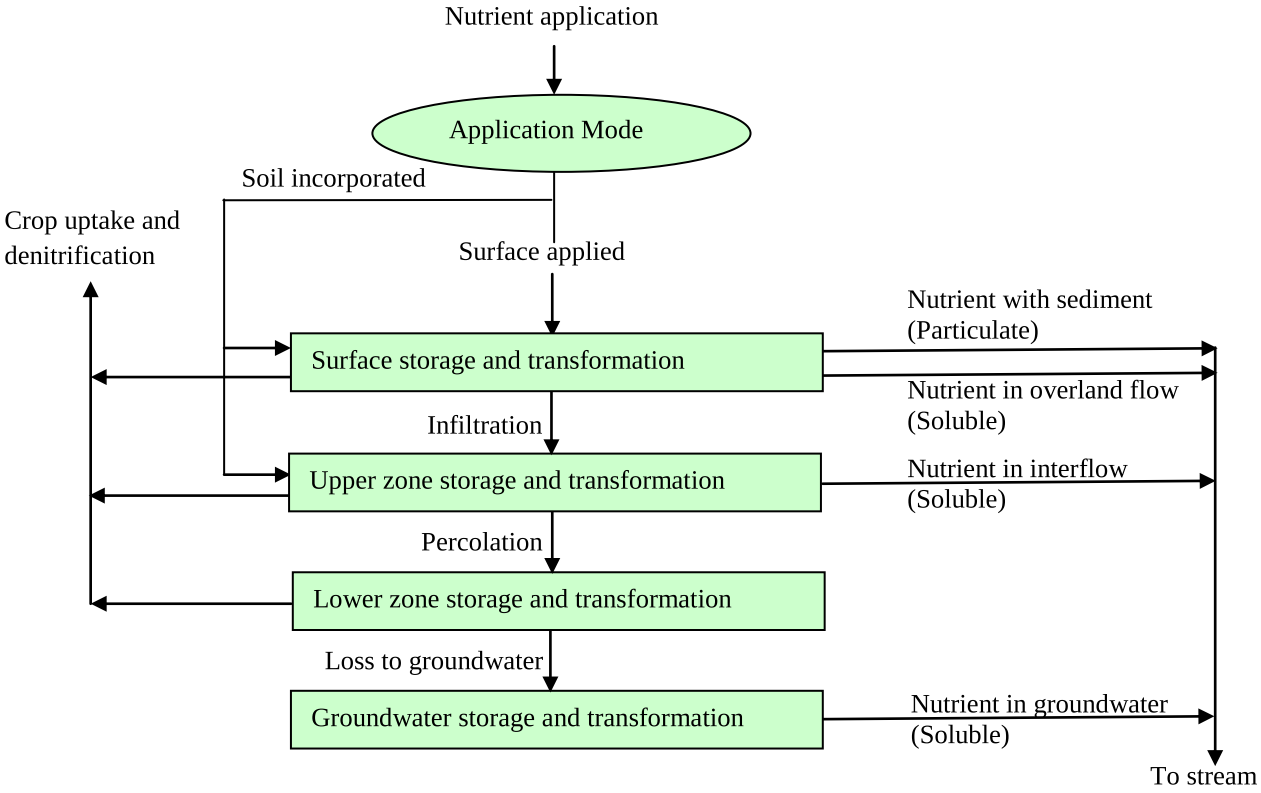


Figure 1: Nutrient Balance Modeled by AGCHEM (modified from Wu, 2004)

Lake Manassas watershed

The Lake Manassas watershed is located in the upper part of the Occoquan watershed in the Northern Virginia suburbs of Washington, DC (Figure 2). The Lake Manassas watershed has a total drainage area of about 123 square miles (189 km^2), covering portions of Fauquier County and Prince William County. The Lake Manassas watershed is a rural watershed undergoing rapid urbanization. Figure 3 shows the 2006 land use map, with data provided by NVRC (Northern Virginia Regional Commission), consolidated into 10 land use categories: forest/idle, golf, pasture, low tillage cropland, high tillage cropland, low density residential, medium density residential, townhouse/garden apartment, institutional, and industrial. In the Lake Manassas watershed, forest/idle has the largest percentage (63.3%) followed by pasture (17.9%). 11.3% of the watershed is urban and residential areas, including industrial, institutional, low density residential, medium density residential and townhouse/garden apartment. High tillage and low tillage croplands cover 6.5% of the watershed. In addition, there are three golf courses located on the north shore of Lake Manassas: Robert Trent Jones International Golf Club, Stonewall Golf Club and the Virginia Oaks Golf Club, covering about 1% of the watershed. Based on the 2002 Census of Agriculture from USDA National Agricultural Statistics Service (NASS) (USDA, 2004), in Fauquier and Prince William counties, the main crops are hay (mostly grown under low tillage condition), corn (almost 50% grown under high tillage condition), wheat (mostly grown under high tillage condition) and soybean (mostly grown under low tillage condition). Using the data from the 2002 Census of Agriculture, county-based cropland distribution of the high tillage and low tillage croplands were estimated (shown in Figure 4). In addition, the major grass grown in the study area is cool season turf grass including tall fescue grass and Kentucky blue grass.

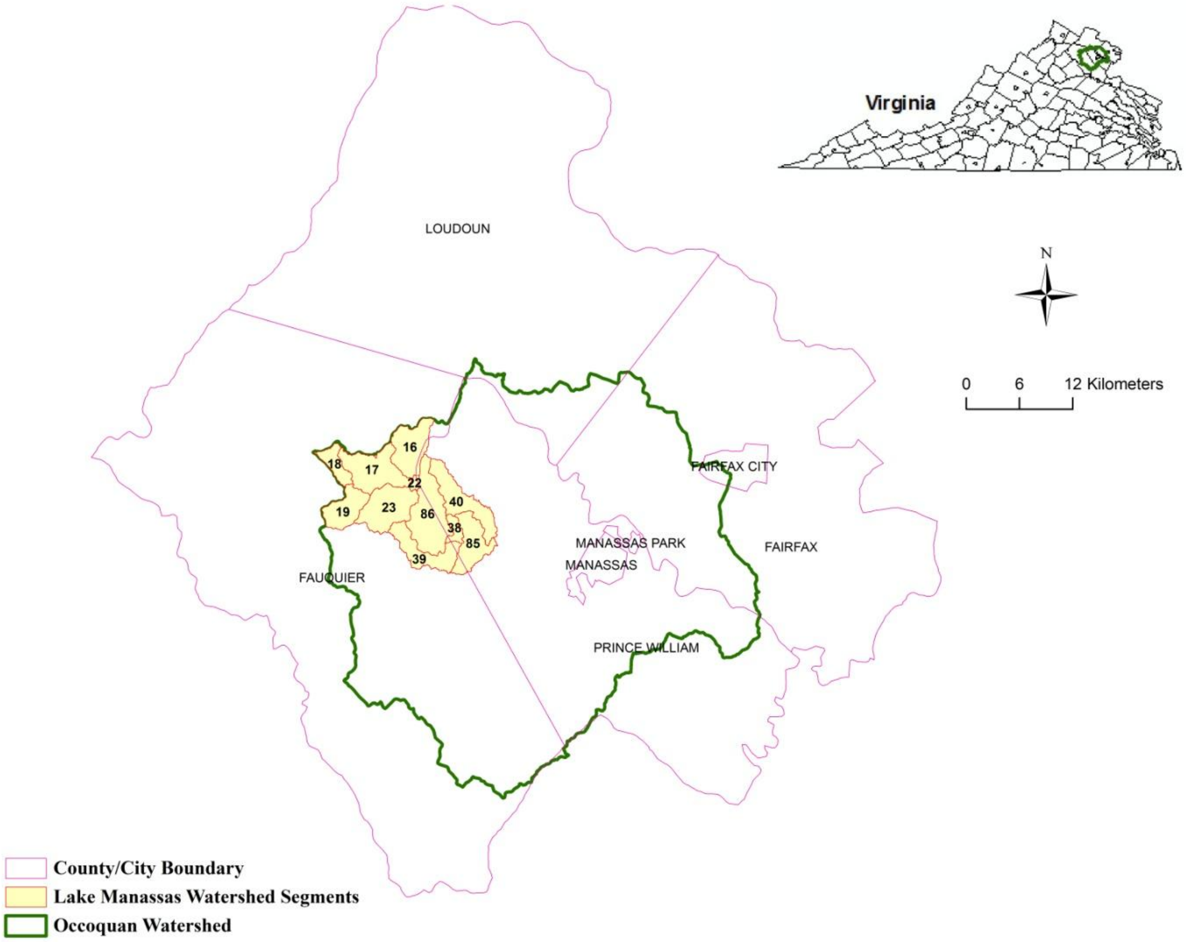


Figure 2: Location of Lake Manassas Watershed, Showing Watershed Segments and Jurisdictional Boundaries

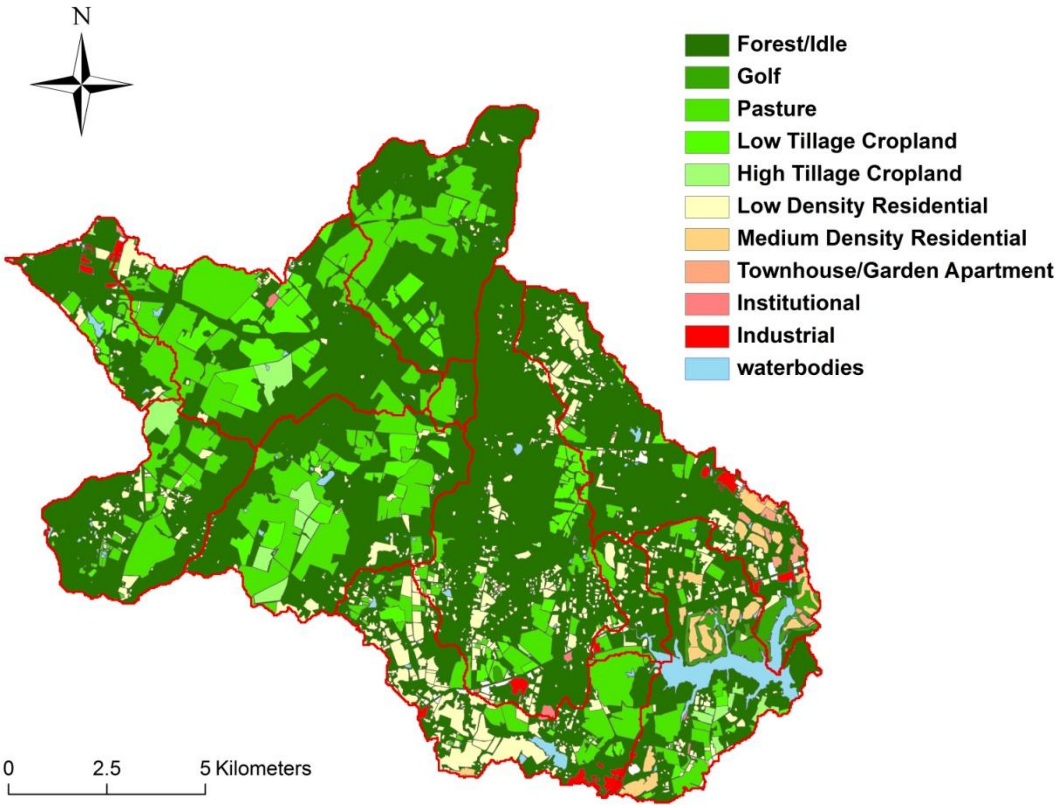


Figure 3: Land Use Map in the Lake Manassas Watershed in 2006 (data from NVRC)

Land use areas for the AGCHEM applications

Nutrient balances within the soil for each vegetation type vary due to factors such as planting and harvesting dates, fertilizer/manure applications, and plant uptake of nutrients. For the AGCHEM applications, the high and low tillage croplands were further split by NVRC into hay, high tillage corn, low tillage corn, wheat, and soybean. These land use areas were estimated based on county-based cropland distribution of the high tillage and low tillage croplands (Figure 4). The cropland distribution is assumed to be uniform throughout a given county. For example, in any land segment falling into Fauquier County, the wheat area is 27% of the high tillage cropland in the segment.

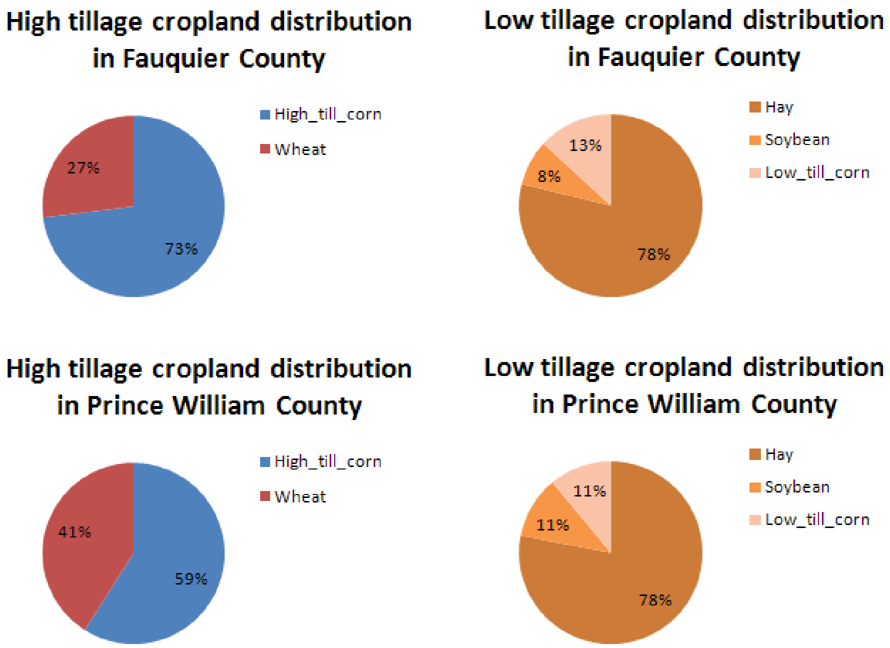


Figure 6: Cropland distribution in Fauquier and Prince William counties

Land use areas for the AGCHEM applications in individual land segments are shown in summary form in Table 1.

Table 1: Land Use Summary for the AGCHEM Applications in Lake Manassas Watershed

Subbasin	Segment	Area (acres)												
		Forest	**Golf**	**Pasture**	**Hay**	**High tillage corn**	**Low tillage corn**	**Wheat**	**Soybean**	**Low density residential**	**Medium density residential**	**Townhouse**	**Institutional**	**Industrial**
Upper Broad Run	16	3472.2	0.0	1193.8	218.4	0.0	36.4	0.0	22.4	45.5	0.0	0.0	0.0	0.0
Upper Broad Run	17	3055.6	0.0	1837.4	743.0	118.6	123.8	43.9	76.2	202.7	0.0	0.0	15.9	21.9
Upper Broad Run	18	1245.2	0.0	263.8	171.6	22.8	28.6	8.4	17.6	117.9	0.0	0.0	13.3	73.5
Upper Broad Run	19	2516.4	0.0	834.5	22.1	111.7	3.7	41.3	2.3	225.6	0.0	0.0	0.0	2.0
Upper Broad Run	22	235.7	0.0	148.4	3.9	0.0	0.7	0.0	0.4	4.3	0.0	0.0	0.0	0.0
Upper Broad Run	23	3290.9	0.0	1721.9	404.3	215.3	67.4	79.6	41.5	235.6	0.0	0.0	0.0	0.0
Upper Broad Run	86	6094.6	19.5	503.6	323.6	8.4	53.9	3.1	33.2	765.2	0.0	0.0	36.5	70.1
Middle Broad Run	72	643.6	0.0	149.7	1.8	0.0	0.2	0.0	0.2	149.4	0.0	0.0	0.0	20.4
Middle Broad Run	73	1992.5	0.0	944.9	64.2	0.0	10.7	0.0	6.6	1203.9	28.9	0.0	7.5	121.6
Middle Broad Run	74	3825.0	200.6	132.6	55.6	0.0	7.8	0.0	7.8	540.2	281.8	127.1	9.5	168.0
Middle Broad Run	85	2373.8	235.8	522.2	71.0	85.1	10.0	59.1	10.0	272.4	379.1	8.1	12.0	46.5
Grand total for Lake Manassas watershed		**28745.4**	**455.8**	**8252.8**	**2079.5**	**561.8**	**343.3**	**235.5**	**218.2**	**3762.8**	**689.9**	**135.2**	**94.5**	**524.1**

Nutrient inputs for the HSPF/AGCHEM applications

Nutrients from fertilizer, manure, and atmospheric deposition were included as inputs for the HSPF/AGCHEM models. The wet and dry atmospheric deposition of NH_4, NO_3 and PO_4 were input as monthly fluxes into the surface soil layer for all land use types. This document focused on estimating the nutrient inputs from fertilizer and manure applications.

For each land use type, the general steps for developing the nutrient inputs included estimating annual nutrient application rates, distributing the annual rates on a monthly basis, and estimating the distribution of monthly nutrients between the surface and upper soil layers. In the study area, the best available data to support the development of the nutrient inputs in the above steps was county-based (Fauquier County and Prince William County), including:

- Crop yields (by county) from USDA National Agricultural Statistics Service (NASS) (USDA, 2004), shown in Table 2.
- Virginia soil test summary (by county) from Virginia Tech Soil Testing Laboratory, shown in Table 3. In the table, phosphorous soil test level (soil P test level) was categorized as L (low), M (medium), H (high) and VH (very high). For each vegetation type in a given county, P rating was represented as the percentage of the soil samples in the four categories (L, M, H and VH).
- Virginia Nutrient Management Standards and Criteria (VDCR, 2005) published by Virginia Department of Conservation and Recreation (DCR) and information supplied by local county DCR.
- Discussions with Virginia Cooperative Extension and local county extension agents (Ohlwiler, 2009; Marshall, 2009).

Table 2: Crop Yields in Fauquier and Prince William Counties (USDA, 2004)

		Crop Yield			
County	**Year**	**Wheat (bushel/acre)**	**Corn (bushel/acre)**	**Soybean (bushel/acre)**	**Hay (ton/acre)**
Fauquier County	2002	53	96	28	1.5
Fauquier County	2003	45	100	37	2.2
Fauquier County	2004	45	131	43	2.5
Fauquier County	2005	39	120	37	2.7
Fauquier County	2006	51	98	42	2.7
Fauquier County	2007	29	91	25	2.4
Fauquier County	**average of the highest three years**	**50**	**117**	**41**	**2.6**
Prince William County	2002	55	47	17	1.3
Prince William County	2003	38	104	27	2.7
Prince William County	2004	48	131	48	2.0
Prince William County	2005	53	105	39	3.2
Prince William County	2006		51	40	1.7
Prince William County	2007		56	16	1.4
Prince William County	**average of the highest three years**	**52**	**113**	**42**	**2.6**

Table 3: Soil Test Summary for P Rating in Fauquier and Prince William Counties (July 1, 2003 – June 30, 2006)

			P Rating			
		Number of samples	**L**	**M**	**H**	**VH**
County	**Vegetation name**		------------------------------%------------------------------			
Fauquier County	Corn	18	56	33	11	0
	Wheat	1	100	0	0	0
	Soybean	3	0	67	33	0
	Tall grass-hay	73	27	37	29	7
	Orchard grass/fescue-clover Pasture	235	32	28	33	7
	Industrial lawns-bluegrass	7	43	29	29	0
	Lawn maintenance-bluegrass	187	28	32	25	16
Prince William County	Corn	4	50	50	0	0
	Tall grass-hay	20	15	45	35	5
	Orchard grass/fescue-clover Pasture	254	45	38	13	4
	Industrial lawns-bluegrass	3	67	0	33	0
	Lawn maintenance-bluegrass	1768	17	34	37	12

Based on the available data, county-based nutrient inputs were developed under the assumption of a typical/representative nutrient application for each land use category in the county. The representative nutrient application was assumed to repeat every year over the entire simulation period. Then, the estimated county-based nutrient inputs were applied to all land segments inside the county. For modeling purposes, the nutrient inputs were specified in the forms of NO_3, NH_4, organic nitrogen, PO_4, and organic phosphorus.

Pasture

Manure was considered as a common source of soil enrichment for pasture. To estimate the amount of manure input to pasture, livestock population data in Fauquier County and Prince William County (Table 4) from the 2002 Census of Agriculture was used.

Table 4: Livestock Population in Fauquier and Prince William Counties (USDA, 2004)

County	**Animal population (head)**					**Pasture area (acres)**
	Beef	**Dairy**	**Poultry (layers > 20 weeks)**	**Swine**	**Sheep**	
Fauquier County	19206	5245	1986	282	866	105277
Prince William County	2321	1325	824	27	119	8911

Based on discussions with a nutrient management specialist at Fauquier County DCR (Marshall, 2009), animals like dairy, poultry and swine are kept mostly in confined areas and such areas in the Lake Manassas watershed were minimal. The beef and sheep were assumed to graze on pasture throughout the year. Since sheep population was minimal compared to beef, manure deposition rates were calculated by dividing the amount of animal waste produced from beef by the acres of pasture. Manure production rates were based on excretion estimates from the USDA Agricultural Waste Management Field Handbook (USDA, 1992). Table 5 shows the waste characterization values for beef.

Table 5: Waste Characterization Values (USDA, 1992)

Animal	Manure produced (lb/d/1000 lb animal)	Avg. animal weight (lb)	Nitrogen produced (lb/d/1000 lb animal)	Phosphorous produced (lb/d/1000 lb animal)
Beef	63	1400	0.33	0.12

The calculated annual and monthly manure nitrogen and phosphorous inputs to pasture in Fauquier County and Prince William County are listed in Table 6. For modeling purposes, the manure nitrogen is further split between organic nitrogen and NH_4 in a ratio of 55 to 45 percent, and manure phosphorous is assumed to be 50% in organic phosphorous and 50% in PO_4. Then, the developed nutrient inputs from manure are included as monthly fluxes into surface soil layer.

Table 6: Estimated Annual and Monthly Nutrient Inputs to Pasture from Manure

	Manure produced (lb/ac)		Manure nitrogen (lb/ac)		Manure phosphorous (lb/ac)		Manure NH_4 input (lb/ac)		Manure Organic N input (lb/ac)		Manure PO_4 input (lb/ac)		Manure Organic P input (lb/ac)	
Month	**Fauquier**	**Prince William**	**Fauquier**	**Prince William**	**Fauquier**	**Prince William**	**Fauquier**	**Prince William**	**Fauquier**	**Prince William**	**Fauquier**	**Prince William**	**Fauquier**	**Prince William**
JAN	498.81	712.16	2.61	3.73	0.95	1.36	1.18	1.68	1.44	2.05	0.48	0.68	0.48	0.68
FEB	450.54	643.24	2.36	3.37	0.86	1.23	1.06	1.52	1.30	1.85	0.43	0.61	0.43	0.61
MAR	498.81	712.16	2.61	3.73	0.95	1.36	1.18	1.68	1.44	2.05	0.48	0.68	0.48	0.68
APR	482.72	689.19	2.53	3.61	0.92	1.31	1.14	1.62	1.39	1.99	0.46	0.66	0.46	0.66
MAY	498.81	712.16	2.61	3.73	0.95	1.36	1.18	1.68	1.44	2.05	0.48	0.68	0.48	0.68
JUN	482.72	689.19	2.53	3.61	0.92	1.31	1.14	1.62	1.39	1.99	0.46	0.66	0.46	0.66
JUL	498.81	712.16	2.61	3.73	0.95	1.36	1.18	1.68	1.44	2.05	0.48	0.68	0.48	0.68
AUG	498.81	712.16	2.61	3.73	0.95	1.36	1.18	1.68	1.44	2.05	0.48	0.68	0.48	0.68
SEP	482.72	689.19	2.53	3.61	0.92	1.31	1.14	1.62	1.39	1.99	0.46	0.66	0.46	0.66
OCT	498.81	712.16	2.61	3.73	0.95	1.36	1.18	1.68	1.44	2.05	0.48	0.68	0.48	0.68
NOV	482.72	689.19	2.53	3.61	0.92	1.31	1.14	1.62	1.39	1.99	0.46	0.66	0.46	0.66
DEC	498.81	712.16	2.61	3.73	0.95	1.36	1.18	1.68	1.44	2.05	0.48	0.68	0.48	0.68
Yearly	**5873.07**	**8385.14**	**30.76**	**43.92**	**11.19**	**15.97**	**13.84**	**19.76**	**16.92**	**24.16**	**5.59**	**7.99**	**5.59**	**7.99**

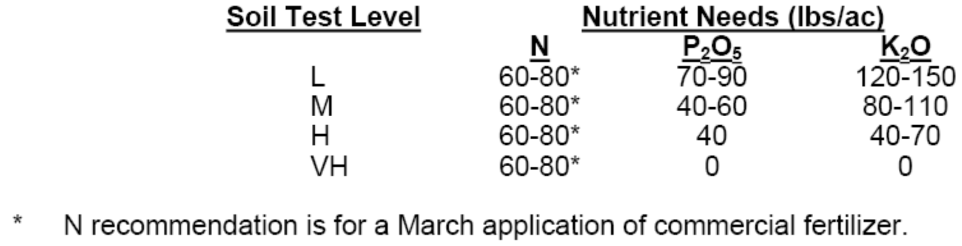
Additional significant nutrient input to pasture is from fertilizer. The fertilizer application is based on Virginia Nutrient Management Standards and Criteria (VDCR, 2005). The publication recommends standard nitrogen application to pasture based on soil productivity group. In this study, the soil productivity group for pasture is determined by pasture carrying capacity (ac/AU): 3.9 in Fauquier County and 2.7 in Prince William County. It is noted that AU is animal unit, representing 1000 lb of any animal type. According to the Virginia Nutrient Management Standards and Criteria (VDCR, 2005), the corresponding soil productivity groups are IV and III in Fauquier County and Prince William County, respectively. For the soil productivity groups IV and III, the recommended nitrogen application for fescue-clover pasture is 40 lb/ac of N (VDCR, 2005).

The estimation of phosphorous application is more complex considering soil P test levels (shown in Table 3). For example, in Fauquier County, 32% of the soil P test results are low, 28% medium, 33% high and 7% very high. According to the Virginia Nutrient Management Standards and Criteria (VDCR, 2005), for fescue-clover pasture in soil productivity group IV, the corresponding P_2O_5 (Phosphorus pentoxide) recommendations for the soil test levels of low, medium, high and very high are 40-60 lb/ac, 30 lb/ac, 0 lb/ac and 0 lb/ac, respectively. Therefore, the P_2O_5 application is calculated as $50\times0.32+30\times0.28=25$ lb/ac. Similarly, the P_2O_5 application in Prince William County is calculated as $50\times0.45+30\times0.38=33$ lb/ac. The fertilizer is mostly applied in August to pasture by surface broadcasting based on the information supplied by a local county DCR official (Marshall, 2009).

Hay

The fertilizer application is based on Virginia Nutrient Management Standards and Criteria (VDCR, 2005), similar to pasture. For hay, however, the soil productivity group is determined by county-based expected yields, shown as the average of the highest three years during the simulation period in Table 2. In both counties, the soil productivity group for hay is determined to be IV. According to the Virginia Nutrient Management Standards and Criteria, for soil productivity group IV, the recommended nitrogen and phosphorous application for fescue (tall grass) hay are listed in Table 7.

Table 7: Recommended fertilizer application rates for fescue (tall grass) hay, soil productivity groups III, IV (VDCR, 2005)



Soil Test Level	Nutrient Needs (lbs/ac)		
	N	P_2O_5	K_2O
L	60-80*	70-90	120-150
M	60-80*	40-60	80-110
H	60-80*	40	40-70
VH	60-80*	0	0

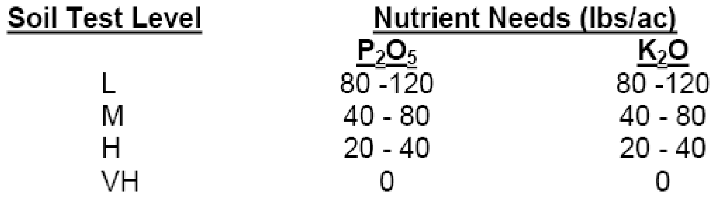
* N recommendation is for a March application of commercial fertilizer.

Then, based on the soil P test levels for tall grass hay (shown in Table 3) and discussions with a local nutrient management specialist (Marshall, 2009), in both counties, the estimated nitrogen application is 80 lb/ac and phosphorous application is 50 lb/ac. In addition, the fertilizer is applied in March by surface broadcasting.

Corn

The fertilizer application is based on Virginia Nutrient Management Standards and Criteria (VDCR, 2005), similar to hay. Based on the county-level expected corn yields in Table 2, the soil productivity group for corn is determined to be IVa in both Fauquier and Prince William counties. According to the Virginia Nutrient Management Standards and Criteria, for soil productivity group IVa, the recommended nitrogen application for corn is 120 lb/ac. Based on discussions with a local nutrient management specialist (Marshall, 2009), 30 lb/ac nitrogen is applied as a starter fertilizer in April by soil incorporation technique. The remaining 90 lb/ac nitrogen is applied in May by surface broadcast. The phosphorous application rate is calculated based on county-level soil P test levels for corn (shown in Table 3) and phosphorous recommendation listed in Table 8. In both counties, the calculated phosphorous application rate is 60 lb/ac. Typically, the 60 lb/ac phosphorous is applied in April, with half of the application by surface broadcast and the other half by soil incorporation technique.

Table 8: Recommended P_2O_5 application rates for corn, soil productivity groups III, IV, V (VDCR, 2005)



Soil Test Level	Nutrient Needs (lbs/ac)	
	P_2O_5	K_2O
L	80 -120	80 -120
M	40 - 80	40 - 80
H	20 - 40	20 - 40
VH	0	0

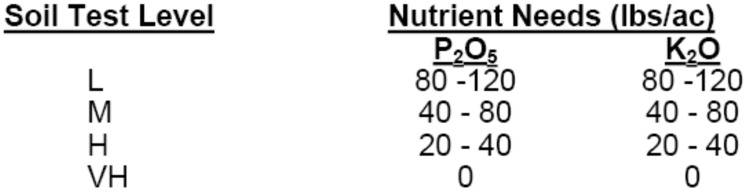
Wheat

The fertilizer application is based on Virginia Nutrient Management Standards and Criteria (VDCR, 2005) as well as discussions with a local nutrient management specialist (Marshall, 2009), similar to corn. However, there is only one soil sample in Fauquier County and no soil sample in Prince William County for wheat. Therefore, the phosphorous application rate is fully dependent on the specialist's personal experience. In both Fauquier and Prince William counties, the recommended nitrogen application for wheat is 100 lb/ac, with 30 lb/ac nitrogen applied as a starter fertilizer in September by surface broadcast and the remaining 70 lb/ac nitrogen applied in February by surface broadcast. In addition, the recommended phosphorous application is 50 lb/ac in September by surface broadcast.

Soybean

Generally, nitrogen fertilizer is not required for soybean since it is a leguminous crop. Phosphorous application rate for soybean is estimated based on soil P test levels (shown in Table 3) and recommended phosphorous application rates listed in Table 9. The calculated phosphorous application rate in Fauquier County is 50 lb/ac. Since there is no soil sample for soybean in Prince William County, the same phosphorous application of 50 lb/ac is used in the study. Based on personal communication with a nutrient management specialist (Marshall, 2009), the 50 lb/ac phosphorous is applied in May by surface broadcasting.

Table 9: Recommended P_2O_5 application rates for soybean, all productivity groups (VDCR, 2005)

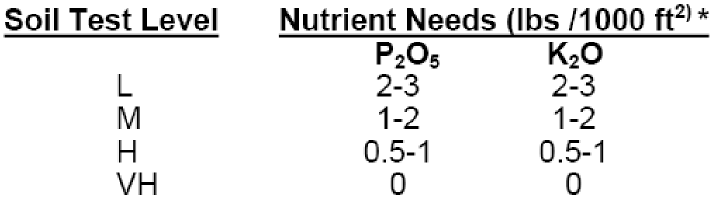


Soil Test Level	Nutrient Needs (lbs/ac)	
	P_2O_5	K_2O
L	80 -120	80 -120
M	40 - 80	40 - 80
H	20 - 40	20 - 40
VH	0	0

Industrial/Institutional

The pervious industrial/institutional areas account for parks, lawns, and areas in which water is able to percolate through the soil. The fertilizer application is developed for the major grass grown in these area: cool season turf grass including tall fescue grass and Kentucky blue grass. According to Virginia Nutrient Management Standards and Criteria (VDCR, 2005) as well as a local extension agent (Ohlwiler, 2009), nitrogen application for both grasses is 2-3.5 lb/1000 ft^2, with a typical distribution of 14.5%-28.5%-28.5%-28.5% (sum = 100%) for May-September-October-November. Phosphorous application rate is estimated based on soil P test levels (shown in Table 3) for industrial lawns-bluegrass and phosphorous recommendation listed in Table 10.

Table 10: Recommended P_2O_5 application rates for established turf (VDCR, 2005)



Soil Test Level	Nutrient Needs (lbs /1000 $ft^{2)}$ *	
	P_2O_5	K_2O
L	2-3	2-3
M	1-2	1-2
H	0.5-1	0.5-1
VH	0	0

Based on the above data, the calculated nitrogen application rate in both Fauquier County and Prince William County is 87 lb/ac. The calculated phosphorous application rate is 56 lb/ac in Fauquier County and 65 lb/ac in Prince William County. However, according to the local nutrient management specialist's personal experience (Marshall, 2009), these numbers are somehow higher in the study area. One possible reason might be that the soil samples mostly cover where intensive turf management practices are applied. A portion of the pervious industrial/institutional areas might have little or no turf maintenance without much fertilizer application. Considering this, the recommended fertilizer application rate for industrial/institutional land uses is adjusted to be 80 lb/ac nitrogen and 40 lb/ac phosphorous in both counties. In addition, the recommended fertilizer application technique for lawns is surface broadcast.

Low density residential/Medium density residential/Townhouse

The nutrient inputs to low density residential/medium density residential/townhouse are similar to industrial/institutional land uses: 2-3.5 lb/1000 ft^2 nitrogen application and phosphorous recommendation shown in Table 10 for home lawns, with a mixed cool season tall fescue grass and Kentucky blue grass. Based on the above data, county-level soil P test levels (shown in Table 3) for lawn maintenance-bluegrass, and personal communication with a local nutrient management specialist (Marshall, 2009), the recommended fertilizer application rate for low density residential/medium density residential/townhouse land uses is 70 lb/ac nitrogen and 30 lb/ac phosphorous in both Fauquier County and Prince William County.

Golf course

The fertilizer application is based on Virginia Nutrient Management Standards and Criteria (VDCR, 2005) as well as 1996 fertilizer application data supplied by Robert Trent Jones Golf Club. While using the Virginia Management Standards and Criteria, the cool season turf grass under intensive management is assumed. Under this assumption, the recommended nitrogen application rate is: total annual N rates of 3-4 lb/1000 ft^2, and maximum N rate per application of 0.5 lb/1000 ft^2. According to the Virginia Management Standards and Criteria, the beginning and ending dates for nitrogen application are determined by the average dates of last killing frost in Spring and first killing frost in Fall. In the study area, the corresponding dates are April 5th and October 30th. In addition, based on the 1996 fertilizer application data on Robert Trent Jones Golf Club, the fertilizer was mostly applied from April through October. Therefore, a total recommended nitrogen application rate of 152 lb/ac is evenly split into seven months (April to October) with a nitrogen rate of 21.8 lb/ac per application. Phosphorous application is indirectly estimated from the nitrogen recommendation based on assumed 3-1-2 ratio “turf-type” fertilizer. That is, a total annual application of 51 lb/ac phosphorous with a monthly distribution of 7.3 lb/ac from April to October.

For each land use type, the recommended fertilizer applications including application rate, timing and technique need to be manipulated for modeling purposes:

- First, the nutrients must enter the model in one of the specific forms: NO_3, NH_4, organic nitrogen, PO_4, and organic phosphorus. For simplification, 25% of nitrogen application is assumed to be converted into NO_3, 75% of nitrogen application is assumed to be converted into NH_4, and 100% of phosphorus application is assumed to be converted into PO_4.
- Second, the nutrient inputs must be specified as being applied to one of the particular soil layers: surface or upper. This depends on the recommended nutrient application technique, i.e., surface broadcasting, and soil incorporation. With surface broadcasting, fertilizer will be applied to the surface layer. With the soil incorporation technique, 10% of the fertilizer will be applied to the surface layer and the remaining 90% will be incorporated into the upper layer based on the assumption that incorporation would produce an approximately uniform distribution of nutrient in the top two soil layers (Donigian et al., 1994).

Based on the above assumptions, the developed NH_4, NO_3 and PO_4 inputs from fertilizer for each land use are included as monthly fluxes into surface and/or upper soil layers, shown in Table 11, 12 and 13.

Table 11: Developed NH_4 inputs from fertilizer for each land use (lb/ac)

Month	Pasture		Hay		Corn		Wheat		Soybean		Industrial/ Institutional		Low density residential/ Medium density residential/Townhouse		Golf course	
	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer
January	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
February	-	-	-	-	-	-	52.5	-	-	-	-	-	-	-	-	-
March	-	-	60.0	-	-	-	-	-	-	-	-	-	-	-	-	-
April	-	-	-	-	2.3	20.2	-	-	-	-	-	-	-	-	16.4	-
May	-	-	-	-	67.5	-	-	-	-	-	8.7	-	7.5	-	16.4	-
June	-	-	-	-	-	-	-	-	-	-	-	-	-	-	16.4	-
July	-	-	-	-	-	-	-	-	-	-	-	-	-	-	16.4	-
August	30.0	-	-	-	-	-	-	-	-	-	-	-	-	-	16.4	-
September	-	-	-	-	-	-	22.5	-	-	-	17.1	-	15.0	-	16.4	-
October	-	-	-	-	-	-	-	-	-	-	17.1	-	15.0	-	16.4	-
November	-	-	-	-	-	-	-	-	-	-	17.1	-	15.0	-	-	-
December	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	**30.0**		**60.0**		**90.0**		**75.0**		**-**		**60.0**		**52.5**		**114.5**	

Table 12: Developed NO3 inputs from fertilizer for each land use (lb/ac)

Month	Pasture		Hay		Corn		Wheat		Soybean		Industrial/ Institutional		Low density residential/ Medium density residential/Townhouse		Golf course	
	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer
January	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
February	-	-	-	-	-	-	17.5	-	-	-	-	-	-	-	-	-
March	-	-	20.0	-	-	-	-	-	-	-	-	-	-	-	-	-
April	-	-	-	-	0.8	6.7	-	-	-	-	-	-	-	-	5.5	-
May	-	-	-	-	22.5	-	-	-	-	-	2.9	-	2.5	-	5.5	-
June	-	-	-	-	-	-	-	-	-	-	-	-	-	-	5.5	-
July	-	-	-	-	-	-	-	-	-	-	-	-	-	-	5.5	-
August	10.0	-	-	-	-	-	-	-	-	-	-	-	-	-	5.5	-
September	-	-	-	-	-	-	7.5	-	-	-	5.7	-	5.0	-	5.5	-
October	-	-	-	-	-	-	-	-	-	-	5.7	-	5.0	-	5.5	-
November	-	-	-	-	-	-	-	-	-	-	5.7	-	5.0	-	-	-
December	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	**10.0**		**20.0**		**30.0**		**25.0**		**-**		**20.0**		**17.5**		**38.2**	

Table 13: Developed PO4 inputs from fertilizer for each land use (lb/ac)

Month	Pasture		Hay		Corn		Wheat		Soybean		Industrial/ Institutional		Low density residential/ Medium density residential/Townhouse		Golf course	
	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer	Surface layer	Upper layer
January	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
February	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
March	-	-	21.8	-	-	-	-	-	-	-	-	-	-	-	-	-
April	-	-	-	-	14.4	11.8	-	-	-	-	-	-	-	-	3.2	-
May	-	-	-	-	-	-	-	-	21.8	-	2.5	-	2.0	-	3.2	-
June	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3.2	-
July	-	-	-	-	-	-	-	-	-	-	-	-	-	-	3.2	-
August	10.9/14.4*	-	-	-	-	-	-	-	-	-	-	-	-	-	3.2	-
September	-	-	-	-	-	-	21.8	-	-	-	5.0	-	3.7	-	3.2	-
October	-	-	-	-	-	-	-	-	-	-	5.0	-	3.7	-	3.2	-
November	-	-	-	-	-	-	-	-	-	-	5.0	-	3.7	-	-	-
December	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
Total	**10.9/14.4***		**21.8**		**26.2**		**21.8**		**21.8**		**17.5**		**13.1**		**22.3**	

* Data for Fauquier County/Prince William County

References

Bicknell, B.R., Imhoff, J.C., Kittle, J.L., Jobes, T.H., and Donigian, A.S, 2005. Hydrological Simulation Program -Fortran (HSPF). User's manual for release 12.2. U.S.EPA. National Exposure Research Laboratory, Athens, GA.

Donigian, A. S., Bicknell, B. R., Patwardham, A. S., Linker, L. C., and Chang, C., 1994. Chesapeake Bay Program: watershed model application to calculate bay nutrient loadings. U.S. EPA-903-R-94-042, Chesapeake Bay Program Office. U.S.EPA. Annapolis, Maryland.

Donigian, A.S., Bicknell, B.R., Chinnaswamy, R.V., and Deliman, P.N., 1998. Refinement of a Comprehensive Watershed Water Quality Model with Application to the Chesapeake Bay Watershed. Technical Report EL-98-6. U.S. Army Corps of Engineers, Waterways Experiment Station, Vicksburg, MS. 244p.

Liu, Z., 2006. Effective Modeling of Agricultural Practices within Large-scale Hydrologic and Water Quality Simulations. PhD. Dissertation, Mississippi State University.

Marshall, J., 2009. Personal Communication. Fauquier County Soil and Water Conservation District, Virginia.

Ohlwiler, T., 2009. Personal Communication. Fauquier County Cooperative Extension Office, Virginia.

United States Department of Agriculture (USDA), 1992. Agricultural Waste Management Field Handbook. Natural Resources Conservation Service, Washington, DC

U.S. Department of Agriculture (USDA), 2004. National Agricultural Statistics Service. 2002 census of agriculture. Available at http://www.nass.usda.gov/census.

Virginia Department of Conservation and Recreation (VDCR), 2005. Virginia Nutrient Management Standards and Criteria.

Wu, J., 2004. Water-quality-based BMP design approach and uncertainty analysis for integrated watershed management. PhD. Dissertation, University of Virginia.