

ABSTRACT

Title of Thesis: CALIBRATING SHENANDOAH WATERSHED SWAT MODEL
USING A NONLINEAR GROUNDWATER ALGORITHM

Yan Wang, Master of Science, 2011

Directed By: Dr. Kaye Brubaker

Water Resources Engineering

Department of Civil and Environmental Engineering

This study contributes to a project with the Interstate Commission on the Potomac River Basin to build a model of the Potomac watershed using the Soil Water Assessment Tool (SWAT). The 2,937 mi² Shenandoah watershed represents about 40% of the Potomac Basin by area. The model subdivides the Shenandoah watershed into 28 subwatersheds and 489 hydrologic response units. SWAT's linear-reservoir groundwater algorithm is modified into a new non-linear method. Modeled flows are compared to observations (dating from 1996 to 2006) at 15 USGS stream gages. The model is auto-calibrated using the Parameter Estimation Software (PEST), experimenting with options to improve model performance. The best model results are obtained by applying ordinal weights to the observation groups, decreasing from headwaters to outlet, and pre-calibrating the roughness coefficients using empirical equations. The calibrated model will contribute to understanding hydrological processes and predicting the effects of land use and climate change in the watershed.

CALIBRATING SHENANDOAH WATERSHED SWAT MODEL USING A
NONLINEAR GROUNDWATER ALGORITHM

by

Yan Wang

Thesis submitted to the Faculty of the Graduate School of the
University of Maryland, College Park in partial fulfillment
of the requirements for the degree of
Master of Science
2011

Advisory Committee:

Associate Professor Kaye L. Brubaker, Chair

Professor Richard H. McCuen

Research Professor Gerald Galloway

© Copyright by

Yan Wang

2011

ACKNOWLEDGEMENT

During this two-year study and research period, my professors, my family and my friends have given me precious supports. I would like to take this opportunity to thank all these people who contributed to the work and helped me in finishing this thesis.

First of all, I would like to give special thanks to my adviser, Dr. Brubaker, for her ideas and acute insight in researches, and for her patience and kindness in supervising me. I would also like to thank Mr. Jan Ducnuigeen, who has provided me with great technical support in setting up the SWAT model.

I would like to thank Dr. McCuen for his excellent statistics and hydrology classes. I learned a lot and they are really useful in my research. I would also like to thank Dr. Galloway for his great lectures on Water Resources Management and taking the time to help revising this work.

Finally, I would like to thank my family. Thank you for your love and support.

Table of Contents

CHAPTER ONE.....	1
INTRODUCTION	1
1.1 INTRODUCTION OF THE STUDY AREA AND BASIC PROCEDURES.....	1
1.2 INTRODUCTION OF THE PROJECT OBJECTIVES	2
1.3 INTRODUCTION OF THE STUDY AREA	3
1.3.1 Potomac River Basin	3
1.3.2 The Shenandoah River.....	5
CHAPTER TWO	8
LITERATURE REVIEW	8
2.1 INTRODUCTION OF HYDROLOGIC MODELING	8
2.1.1 Watershed.....	8
2.1.2 Hydrologic modeling	9
2.1.3 Current hydrologic modeling environments	10
2.2 INTRODUCTION OF SWAT	12
2.2.1 Basic features of SWAT.....	13
2.2.2 Basic modeling method of SWAT	14
2.2.3 Input and output files for SWAT	19
2.2.4 Modification of the SWAT software	22
2.3 HYDROLOGIC MODEL CALIBRATION	24
2.3.1 Optimization algorithm	24
2.3.2 Automatic calibration of hydrologic models.....	26
2.4 INTRODUCTION OF PEST	27
2.4.1 PEST history.....	27
2.4.2 The PEST optimization method	28
2.4.3 Operations of PEST	29
2.4.4 Termination criteria	31
2.4.5 Hydrologic applications of PEST.....	31
CHAPTER THREE	34
THE NEW GROUNDWATER ALGORITHM	34
3.1 INTRODUCTION OF THE HYDROGRAPH	34

3.2 INTRODUCTION OF BASEFLOW SEPARATION	34
3.2.1 Constant-Discharge Method.....	35
3.2.2 Constant-Slope Method.....	35
3.2.3 Concave Method	36
3.3 SWAT BASEFLOW ALGORITHM	37
3.4 THE NEW BASEFLOW ALGORITHM	40
CHAPTER FOUR	43
MODEL SETUP	43
4.1 WATERSHED DELINEATION	43
4.1.1 Level one: Hydrologic Unit Code	43
4.1.2 Level two: Subwatersheds	44
4.1.3 Level three: Hydrologic Response Units.....	47
4.2 INPUT FILES NEEDED FOR SWAT	49
4.3 INPUT FILES FOR PEST --- COUPLING OF PEST AND SWAT	55
4.3.1 Selection of SWAT parameters for calibration.....	56
4.3.2 Preparing PEST input files	59
4.4 DISCHARGE DATA FOR COMPARISON.....	60
4.5 MODEL SUMMARY	62
CHAPTER FIVE	64
GENERAL METHODS FOR MODEL MODIFICATION AND ANALYSIS	64
5.1 MEASURES OF MODEL PERFORMANCE	64
5.1.1 Parameter rationality.....	65
5.1.2 Goodness of fit of modeled discharge.....	65
5.1.3 Nash-Sutcliffe coefficients	68
5.1.4 Other criteria.....	72
5.2 WEIGHTED OBJECTIVE FUNCTION	74
5.3 INCREASING THE NUMBER OF ADJUSTABLE PARAMETERS.....	79
5.4 SELECTION OF ADJUSTABLE PARAMETERS.....	82
5.5 EXPLORATION MADE WITHIN PEST	89
5.5.1 Using Predictive Analysis Mode in PEST auto-calibration process.....	89
5.5.2 Using Regularization Mode in PEST auto-calibration process.....	91
5.5.3 SENSAN package.....	92

5.6 CHAPTER SUMMARY	94
CHAPTER SIX.....	96
MODEL EXPERIMENTS AND RESULTS	96
6.1 SWAT-PEST MODEL OUTPUT VERSION 2.....	96
6.2 iSWAT-PEST MODEL OUTPUT VERSION 3 MODIFIED	102
6.3 iSWAT-PEST MODEL OUTPUT VERSION 9	106
6.4 NEW ROUGHNESS COEFFICIENTS FOR MAIN CHANNELS.....	111
6.5 iSWAT-PEST MODEL OUTPUT VERSION 16	112
6.6 EVALUATION OF PARAMETER RATIONALITY.....	120
6.7 COMPARISON OF R AND R_w IN ALL MODEL VERSIONS	123
CHAPTER SEVEN	125
CONCLUSION AND DISCUSSION	125
7.1 CONCLUSION.....	125
7.2 FUTURE RESEARCH	128
7.3 LESSONS LEARNED.....	132
APPENDIX A SWAT INPUT FILES LIST	134
APPENDIX B STUDY RECORDS	136
REFERENCES	154

CHAPTER ONE

INTRODUCTION

1.1 INTRODUCTION OF THE STUDY AREA AND BASIC PROCEDURES

This work is part of a project of the Interstate Commission on the Potomac River Basin (ICPRB), which aims at building virtual watershed models for the entire Potomac River Basin. The study area is the Shenandoah River Basin, generally known as the Shenandoah Valley, including the South Fork Shenandoah, the North Fork Shenandoah and the Shenandoah (Lower Shenandoah) watershed.

The model is implemented using the Soil Water Assessment Tool (SWAT) (Neitsch, 2005). In groundwater calculations, SWAT applies a linear-reservoir algorithm. However, with more researches on this assumption and due to observations of baseflow recession in the study area, a new nonlinear algorithm (Wittenberg and Sivapalan, 1999) was introduced in SWAT, creating a new version of SWAT called iSWAT.

This is a continuous work of the already underway project. The modification of SWAT to iSWAT has already been done. My work here is an application of iSWAT, coupling it with automated calibration software and calibrating the watershed model for the Shenandoah Valley. The model-independent Parameter Estimation Tool (PEST) (Doherty, 2004) is applied for calibration. Methods explored are applying different weighting methods, reducing parameter space by pre-calibration of certain parameter values.

This chapter introduces the purpose and physical setting of the model. Chapter Two is a review of the relevant technical literature including brief introduction of watershed analysis, hydrologic modeling, specifics of the SWAT modeling environment, and the PEST calibration package. Chapter Three focuses on the new groundwater algorithm employed in this model. Chapter Four deals with the model setup, input files needed and how the two software packages (SWAT and PEST) are coupled. Chapter Five states the general methods in modifying model performances and criteria for model evaluation. Chapter Six shows the results and related analysis. Chapter Seven draws conclusions for the whole study.

1.2 INTRODUCTION OF THE PROJECT OBJECTIVES

The Interstate Commission on the Potomac River Basin (ICPRB) was established in 1940 to improve water quality and maintain the integrity of the Potomac River Basin. ICPRB's mission is to "enhance, protect, and conserve the water and associated land resources of the Potomac River and its tributaries through regional and interstate cooperation, including the states of Maryland (MD) and West Virginia (WV), the commonwealths of Pennsylvania (PA) and Virginia (VA), and the District of Columbia." (ICPRB, 2011)

In 1982, The Water Supply Coordination Agreement was developed among the Fairfax County Water Authority (FCWA), Washington Suburban Sanitary Commission (WSSC), and the ICPRB. The ICPRB Section for Cooperative Water Supply Operations on the Potomac (CO-OP) was designated by the Water Supply Coordination Agreement to be responsible for coordination of water

resources during times of low flow. The management objectives embodied in the agreement and practiced by CO-OP are to keep the off-Potomac reservoir resources balanced while meeting environmental requirements and municipal demands for water. (ICPRB, 2010)

Given increasing concern about water supply and watershed health, the CO-OP section of ICPRB decided to build a digital model of the Potomac River Basin using an established hydrologic modeling environment. The purpose of the program is to understand the physical processes associated with variability in water supply and the effects of human activities on water supply. More important is to allow more accurate assessment of drought risk, the need for resource development, to predict potential effects of future climate and land use change and to provide implications for management.

1.3 INTRODUCTION OF THE STUDY AREA

1.3.1 Potomac River Basin

The Potomac River Basin is the second largest contributor of fresh water to the Chesapeake Bay. The Potomac River is often called the Nation's River. It runs 383 miles (616 km) from the Fairfax Stone in West Virginia to Point Lookout, Maryland and drains 14,679 square miles (38,020 km²). The average flow is 10,800 ft³/s (306 m³/s). (ICPRB, 2010)

Nearly five million people live in the Potomac River Basin, with 3.5 million of them in the Washington, D.C. metropolitan area. An average of approximately

486 million gallons of water per day (21m³/s) is withdrawn daily in the Washington area for water supply.

People and their activities have challenged the river. Beginning in the 19th century, with increasing mining and agriculture upstream and urban sewage and runoff downstream, the water quality of the Potomac River deteriorated. From acid mine deposition in its headwaters, intensive crop and animal agriculture in the middle tributaries, to growth and development away from the eleven major cities in the basin, each has brought change and impacts on the Potomac River. Aquatic life originally inhabiting the upstream areas has been greatly affected by mining drainage. Agriculture has degraded habitat in riparian areas and deteriorated water quality by high levels of nutrient and sediment loading. Development of cities and changes in land use result in increasing direct runoff, sedimentation, impairment of local streams and higher potential of flooding. (ICPRB, 2008)



Figure 1.1 Potomac Basin (Musser, 2011)

1.3.2 The Shenandoah River

This work focuses on Shenandoah River Basin, including the South Fork Shenandoah, the North Fork Shenandoah and the Shenandoah (Lower Shenandoah) watershed. The region is known as the Shenandoah Valley. The valley is bounded to the east by the Blue Ridge Mountains, to the west by the eastern front of the Ridge-and-Valley Appalachians (excluding Massanutten Mountain), to the north by the Potomac River and to the south by the James River. The cultural region covers a larger area that includes all of the valley plus the Virginia highlands to the west, and the Roanoke Valley to the south. It is physiographically located within the Ridge and Valley province and is a portion of the Great Appalachian Valley. (ICPRB, 2011)

The Shenandoah River Basin encompasses over 2,937 mi² (7,607 km²). This area occupies the counties of Frederick, Rockingham, Shenandoah, Page, Warren, and Clarke, and the cities Harrisonburg, Staunton, Waynesboro, Winchester, and Front Royal in Virginia and Jefferson County in West Virginia. (ICPRB, 2011) This area usually has 35 to 37 inches of rain per year. The average maximum temperature is 66.6°F and the average minimum temperature is 42.1°F. (Southeast Regional Climate Center, 2010)

Virginia's flora and fauna are among the most diverse to be found anywhere in the temperate latitudes. Within the Shenandoah Valley, there are over a hundred threatened, endangered, or sensitive plants and animals designated by the state and/or federal listing. These include the federally endangered Indiana bat, Virginia big-eared bat, and peregrine falcon. (Potomac River Partnership, 2008)

The Shenandoah River has one of the lowest percentages of intact riparian forests and the greatest potential for restoration in the state of Virginia. The primary water quality problems are nutrient and sediment contamination from agricultural uses, stream erosion, and floodplain encroachment. There have been a significant number of insect and disease outbreaks, wildfires, mountain harvesting activities, and growing use conflicts at the urban/wild land interface - including recreational growth through greenways and dispersed recreation (hunting, hiking ORV/ATV use). Recreation use associated with the Shenandoah River is increasing annually, with current use estimated at 250,000 recreation visitor days a year. (Potomac River Partnership, 2008)

Historically, row cropping and cattle grazing, and more recently, chicken and hog farming have occurred on riparian and upland areas. Severe flood events over the last decade have increased attention on the river corridors. Recently completed re-vegetation work has the promise of returning some areas to a native condition and concerted efforts to conserve riparian areas through conservation easements and repair riparian areas along agricultural corridors are showing significant restoration successes. (Potomac River Partnership, 2008)

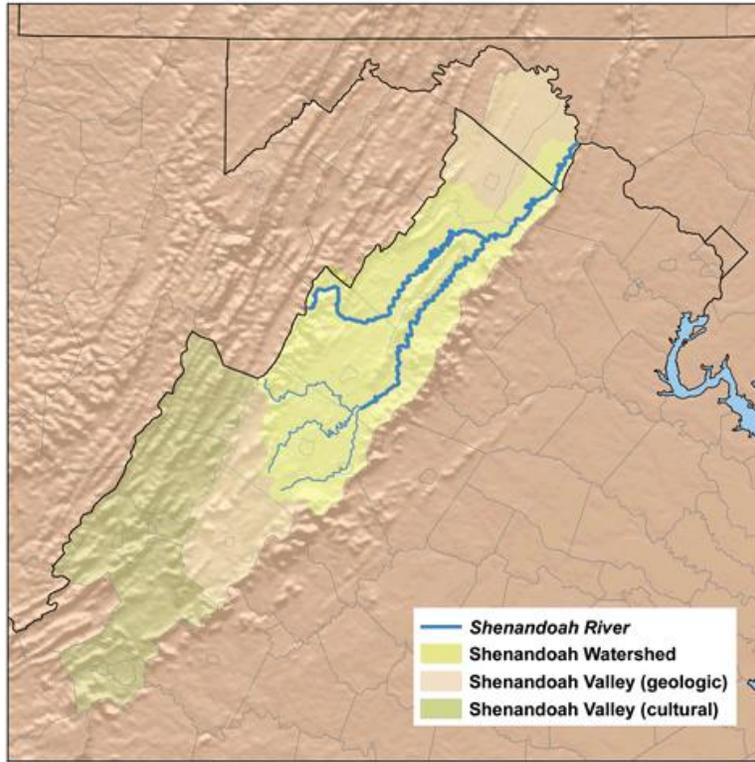


Figure 1.2 Shenandoah Valley (Musser, 2006)

CHAPTER TWO

LITERATURE REVIEW

This chapter first presents a general overview of hydrologic modeling and modeling environments or software. The Soil Water Assessment Tool (SWAT), the modeling environment used in this thesis, is discussed in depth. Next, the principles of model calibration are reviewed, and the automatic calibration tool used in this thesis (PEST) is discussed in detail.

2.1 INTRODUCTION OF HYDROLOGIC MODELING

2.1.1 Watershed

A watershed is an extent or area of land where surface water from rain and melting snow or ice converges to a single point, usually the exit of the basin, where the waters join another water body, such as a river, lake, reservoir, estuary, wetland, sea, or ocean (DeBarry, 2004).

Watersheds come in all shapes and sizes. Some watersheds can be as small as a footprint; some others can be large enough to encompass all the land that drains water into the Chesapeake Bay, where it enters the Atlantic Ocean. They cross county, state, and national boundaries. In the continental US, the US Environmental Protection agency defines 2,110 watersheds; including Hawaii Alaska, and Puerto Rico, there are 2,267 watersheds (USEPA, 2009).

2.1.2 Hydrologic modeling

Models are representations of systems or processes. Some models are actually miniature physical representation of natural systems. Sometimes, series of equations are used to represent the systems, thus forming mathematical models. The number, form, and interconnections of these equations in a model can range from very simple to highly sophisticated. The equations within the mathematical models can be produced from basic physical laws or from statistical analysis of observed data (empirical equations). (Butcher, 2008)

Watershed models simulate natural processes of the flow of water, sediment, chemicals, nutrients, and microbial organisms within watersheds, as well as quantify the impact of human activities on these processes (Butcher, 2008). These models play an important role in predicting water quantity and water quality, two key elements in watershed resources study. Researchers and engineers use model predictions to make decisions on engineering projects such as flood control, wetland restoration, and dam operation.

The Stanford Watershed Model, developed in 1959, was the first integrated attempt to take advantage of the advent of digital computers to describe quantitatively the hydrologic processes that take place in a watershed “within the limitation of current understanding and the limitations of the computer” (Duan, 2002). With more understanding of the physics about watershed and increasing computational power, many complex modeling environments have been developed.

2.1.3 Current hydrologic modeling environments

Current watershed models can be divided into two categories in general, lumped models and distributed models.

Lumped models are systems where all of the parameters that impact the hydrologic response of a watershed are spatially averaged together to represent the basin as a whole. Lumped models assume uniform rainfall and uniform watershed characteristics such as soil types, vegetation types, and land-use practices. Lumped models consider a watershed catchment as one complete unit, characterized by a relative small number of parameters and variables (Shultz, 2007).

Distributed models use parameters that are directly related to the physical characteristics of the basin. These models take into account the spatial variability of both input and output hydrologic variables for a given watershed, and the hydrologic response at ungauged sites within the basin. Distributed models may also account for the spatial variability of the meteorological conditions of the drainage basin (Shultz, 2007).

The current generation of watershed modeling environments (which modelers use to build watershed models) is quite diverse and varies significantly in sophistication and data and computational requirements. Newly emerging technologies are being increasingly integrated into watershed models. According to parameter features and main functions, current hydrologic modeling environments are classified as (TAMU, 2011):

a) Distributed models:

3D-Catchment Conceptual Multilayer Model (ArcEGMO), Bochum Water Balance Model (BWBM), CEQUEAU, Central Valley Groundwater and Surface water model (C2VGSM), Dynamic Watershed Simulation Model (DWSM), Hydrological River Basin Environment Assessment Model (HydroBEAM), Integrated Water Flow Model (IWFM), Kinematic Runoff and Erosion Model, Version 2 (KINEROS2), Physically-Based Distributed Erosion Model (MEFIDIS), One-Dimensional Numerical Model (SVAT-HYCY), Storm Water Management Model (SWMM)

b) Lumped and Parametric Models

Geomorphology-Based Hydrological Model (GBHM), Hydrologic Modeling System (HEC-HMS), Hydrologic Simulation Model (HSIMHYD), Integrated Hydro Meteorological Model (IHMM), Illinois Urban Catchment Runoff Simulation (ILUCAT), Large Basin Runoff Model (LBRM), Rainfall-Runoff Modeling Toolbox (RRMT) & Monte-Carlo Analysis (RRMT&MCAT), Soil Conservation Service Curve Number Model (SCS-CN), SIRMODII, Soil-Plant-Air-Water System (SPAW), Hydrograph Simulation Model (SYN-HYD), Utah Energy Balance Snowmelt Model (UEB), Hydrological Model and Forecasting System (WATFLOOD), Watershed Bounded Network Simulation Model (WBNM), Mathematical Model for Rainfall-Runoff Transformation (WISTOO)

c) Environmental Models

Agricultural Non-Point Source Pollution Models (AGNPS 98), Areal Nonpoint Source Watershed Environmental Simulation (ANSWERS), Erosion

Productivity-Impact Calculator/ Environmental Policy Integrated Climate (EPIC), Hydrologic Simulation Program-Fortran (HSPF), LOAD ESTimator (LOADEST), Illinois Least-Cost Sewer System Design Model (ILSD), Illinois Urban Storm Runoff Model (IUSR), Water Quality/Solute Transport (OTIS), Soil Water Assessment Tool (SWAT), Large Scale Catchment Model, formerly CALSIM (WRIMS).

d) Monthly Water Balance Models

Two-Parameter Water Balance Model (TPWBM), Truckee - Carson Water Operations Model, Water Balance Simulation Model (WASMOD).

e) Real Time Flow Forecasting Models

National Weather Service River Forecast System (NWSRFS), Watershed Bounded Network Model (WBNM2007).

Though there are many hydrologic models and they are constantly improving, models are just a type of tool, and can be used in combination with many other assessment techniques. Models are a reflection of our understanding of watershed system. As with any tool, the answers they give are dependent on how modelers apply them, and the quality of these answers is no better than the quality of our understanding of the system (Butcher, 2008).

2.2 INTRODUCTION OF SWAT

Soil and Water Assessment Tool (SWAT) is a river basin, or watershed scale model developed by Dr. Jeff Arnold in 1985 for the USDA Agricultural Research

Service. SWAT was developed to predict the impact of land management practices on water, sediment and agricultural chemical yields in large complex watersheds with varying soils, land use and management conditions over long periods of time. ArcSWAT, a version of SWAT integrated with a Geographic Information System (Winchell, 2007) allows the user to prepare SWAT input and run the model within the framework of ArcGIS (Winchell, 2007).

2.2.1 Basic features of SWAT

SWAT is a continuous time, long-term yield spatially discrete model. The model is not designated for single-event flood routing. Compared to other modeling environment, SWAT has some unique features (i through iv quoted from SWAT Manual, Neitsch, 2005):

- i. SWAT is process based. Rather than incorporating regression equations to describe the relationship between input and output variables, SWAT requires specific information about weather, soil properties, topography, vegetation, and land management practices occurring in the watershed. The physical processes associated with water movement, sediment, crop growth, nutrient cycling, etc. are directly modeled by SWAT using input data.
- ii. SWAT uses readily available inputs. While SWAT can be used to study more specialized processes such as bacteria transport, the minimum data required to make a run are commonly available from

- the government agencies, such as precipitation and temperature data.
- iii. SWAT is computationally efficient. Simulation of very large basin or a variety of management strategies can be performed without excessive investment of time or money.
 - iv. SWAT enables users to study long-term impacts. Many of the problems currently addressed by users involve the gradual buildup of the pollutants and the impact on downstream water bodies. To study these types of problems, results are needed from runs without output spanning several decades. (Neitsch, 2005)

2.2.2 Basic modeling method of SWAT

Conservation of mass is the basic principle of hydrologic modeling. Simulation of the hydrology of a watershed can be separated into two major divisions. The first division is the land phase of the hydrology cycle. The land phase of the hydrologic cycle controls the amount of water, sediment, nutrient and pesticide loading to the main channel in each subbasin. The second division is the routing phase of the hydrologic cycle, which can be defined as the movement of water, sediments, etc. through the channel network of the watershed to the outlet. (Neitsch, 2005)

In SWAT, watersheds are divided into subbasins and each subbasin is further divided into numbers of Hydrologic Response Units (HRU). The division of the subbasins is determined by geological location and connection of the streams.

The classification of HRU is determined by soil types, land used conditions, and elements related to vegetation and landscape characteristics. Each HRU is spatially independent. Water generated from HURs contributes to reaches through the most upstream end of the main river within the subbasin. Subbasins are spatially connected by river reaches. Water contributed to each subbasin is then conveyed through reaches along the stream network.

The land phase generally represents the water cycles within subbasins and the routing phase represents the water flow among subbasins.

2.2.2.1 The land phase of hydrologic cycle in SWAT

Note: This section is quoted and quoted and summarized from SWAT Manual (Neitsch, 2005)

1) Water Balance

The land phase of the hydrologic cycle simulated by SWAT is based on the water balance equation:

$$SW_t = SW_o + \sum_{i=1}^t (R_{day} - Q_{surf} - E_a - w_{seep} - Q_{gw}) \quad Eq. 2.1$$

where t is the time, i is the time index;

SW_t is the final soil water content on day i;

SW_o is the initial soil water content on day i,

R_{day} is the amount of precipitation on day i,

Q_{surf} is the amount of surface runoff on day i,

E_a is the amount of evaporation on day i,

w_{seep} is the amount of water entering the vadose zone from the soil profile on day i ,

Q_{gw} is the amount of return flow on day i .

2) Modules

Each module indicates one set of processes, including external forcing and system properties. External forcing includes climate and land use (management). System properties are specified using parameters.

i. Climate

The climate of a watershed provides the moisture and energy inputs that control the water balance and determine the relative importance of the different components of the hydrologic cycle. The variables required by SWAT consist of daily precipitation, maximum/ minimum air temperature, solar radiation, wind speed and relative humidity,

ii. Hydrology

As precipitation descends, it may be intercepted and held in the vegetation canopy or fall to the soil surface. Water on the soil surface will infiltrate into the soil profile or flow overland as runoff. Runoff moves relatively quickly toward the stream channel and contributes to short-term stream response. Infiltrated water may be held in the soil and later evaporated or transpired, or it may slowly make its way to the surface water system via underground paths contributing to delayed event response or baseflow.

iii. Land Cover

SWAT utilizes a single plant growth model to simulate all types of land cover. The model is able to differentiate between annual and perennial plants. The plant growth model is used to assess removal of water and nutrients from the root zone, transpiration, and biomass/yield production.

iv. Erosion

Erosion and sediment yield are estimated for each Hydrologic Response Unit with the Modified Universal Soil Loss Equation (MUSLE). MUSLE uses the amount of runoff to simulate erosion and sediment yield. The hydrology model supplies estimates of runoff volume and peak runoff rate which, with the subbasin area, are used to calculate the runoff erosive energy variable.

v. Nutrients

SWAT tracks the movement and transformation of several forms of nitrogen (N) and phosphorus (P) in the watershed. The different forms of N and P are subjective to transport solution, transport with sediments, uptake by plants, and other processes. Nutrients may be introduced to the main channel and transported downstream through surface runoff and lateral subsurface flow.

vi. Pesticides

SWAT simulates pesticide movement into the stream network via surface runoff, and into the soil profile and aquifer by percolation. The movement of the pesticide is controlled by its solubility, degradation half-life, and soil organic carbon adsorption coefficient to the appropriate half-life. Pesticide transport by water and sediment is calculated for each runoff event and pesticide leaching is estimated for each soil layer when percolation occurs.

vii. Management

SWAT allows the user to define management practices taking place in every HRU. The user may define the beginning and the ending of the growing season; specify timing and amount of fertilizer, pesticide and irrigation applications as well as timing of tillage operations. At the end of the growing season, the biomass may be removed from the HRU as yield or placed on the surface as residue.

In addition to these basic management practices, operations such as grazing, automated fertilizer and water applications, and incorporation of management option for water use are available. The latest improvement to land management is the incorporation of routines to calculate sediment and nutrient loading from urban areas (Neitsch, 2005).

2.2.2.2 The routing phase of hydrologic cycle in SWAT

Note: This section is quoted and quoted and summarized from SWAT Manual (Neitsch, 2005)

Once SWAT determines the loading of water, sediment, nutrients and pesticides to the main channel, the flows and loads are routed through the stream network. In addition to keeping track of mass flow in the channel, SWAT simulates the transformation of chemicals in the stream and streambed.

i. Routing the main channel

Routing in the main channel can be divided into four components: water, sediment, nutrients and organic chemicals.

Flow is routed through the channel using a variable storage coefficient method or the Muskingum Routing Method (Neitsch, 2005). SWAT uses stream power to estimate deposition/ degradation, which controls the transport of sediment in the channel. Nutrient transformations in the stream are controlled by the in-stream water quality component of the model. The total pesticide load in the channel is partitioned into dissolved and sediment-attached component, which are transported with water and affected by sediment transport/ deposition respectively.

ii. Routing in the reservoir

The water balance for reservoirs includes inflow, outflow, rainfall on the surface, evaporation, seepage from the reservoir bottom and diversions. In the Shenandoah iSWAT model, no wetland/ reservoir is included.

2.2.3 Input and output files for SWAT

Note: This section is quoted and quoted and summarized from SWAT Manual (Neitsch, 2005)

2.2.3.1 Input files

Input for SWAT is defined at one of several different levels of detail: watershed, subbasin, and HRU. Unique features such as reservoirs or point sources must

have input data provided for each individual feature included in watershed simulation.

Watershed level inputs are used to model processes throughout the watershed. Subbasin level inputs are inputs set at the same value for all HRUs in the subbasin if the input pertains to a process modeled in the HRU. HRU level inputs are inputs that can be set to unique values for each HRU in the watershed.

Besides the files that contain the specific data, there are also files required to control all the input and output files. These include,

- FILE.cio --- master control input/output file. This file dictates the simulation start and end times, and whole-basin-level input files that are read at various stages of execution. In particular, File.cio directs model execution to the weather input files and the model configuration file, *.fig. Different versions of .cio are required to run different models. These are stored as modelname.cio, and the appropriate one must be copied to FILE.CIO before ISWAT_2008c is run.
- Runname.fig --- configuration file. This control file dictates the model topology (connectedness) of subbasins and reaches. In addition, it specifies the subbasin-level files *.sub, *.rte, and *.swq that will be called. The ArcSWAT preprocessor creates .fig files for the separate HUCs, for example (renamed to):SFShen.fig, NFShen.fig, and LowerShen.fig.
- Each subbasin needs 3 required input files, and each HRU needs 4 required input files.

Other input files are listed in the table in Appendix A.

2.2.3.2 Output files

A number of output files are generated in every SWAT simulation: the summary input file (input.std), the summary output file (output.std), the HRU output file (output.hru), the subbasin output file (output.sub), and the main channel or reach output file (output.rch).

- The input summary file prints summary tables of important input values. This file provides the user with a mechanism to spot-check input values. All model inputs are not printed, but the file does contain some of the most important.
- The output summary file provides watershed average loadings from the HRUs to the streams. Tables are also included that present average annual HRU and subbasin values for a few parameters.
- The HRU output file contains summary information for each of the hydrologic response units in the watershed. The file includes date, area, precipitation, flow conditions, evaporation, water quality and other variable values being simulated for each HRU.
- The subbasin output file contains summary information for each subbasin in the watershed. The reported values for the different variables are the total amount or weighted average of all HRUs within the subbasin.
- The main channel output file contains summary information for each routing reach in the watershed. The files include variable values such as average daily stream flow, evapotranspiration, sediment transported, nitrogen transported and etc.

- The HRU impoundment output file contains summary information for ponds, wetlands and depressional areas in the HRUs.
- The reservoir output file contains summary information for reservoirs in the watershed. (Neitsch, 2005).

2.2.4 Modification of the SWAT software

SWAT, a semi-distributed modeling environment, is widely used in modeling water quantity and water quality. Although SWAT is powerful enough to model almost all characteristics in different watersheds, modification of the program itself is sometimes needed to accommodate special cases and situations in each watershed. The SWAT developers make the FORTRAN source code available for users who wish to modify it (Official SWAT Web Site, 2011).

By adding a snowfall–snowmelt routine for mountainous terrain in SWAT, Fontaine (2002) was able to make SWAT to simulate hydrology of a non-agricultural mountainous region with a large snowmelt component.

Vazquez-Amabile (2005) expanded SWAT's capabilities to compute perched groundwater table depth. Van Griensven (2005) used a time step of a user-defined fraction of an hour and an hourly time step to calculate the rainfall/runoff and the in-stream river routing processes, respectively. And he further improved the hydrologic module by including a convolution module and modifications of the evapotranspiration module of SWAT.

Tolson and Shoemaker (2007) modified the input files for SWAT 2000 in order to account for excess soil water movement in frozen soils in Cannonsville Reservoir Watershed.

Baffaut and Benson (2008) modified the SWAT 2005 code to simulate faster aquifer recharge in Karst environments for the James River Basin in Southwest Missouri. Echegaray (2009) further modified the SWAT-Karst to represent Karst environments at the HRU scale. Liu and Yang (2008) used a mass balance algorithm and created an SWAT extension which can simulate riparian wetlands hydrologic processes.

To develop a distributed hydrological cycle model of an irrigation district, Zheng (2010) modified the SWAT model in the aspects of the extraction of ditches, distributed subbasins and hydrologic response units, and the calculation method of the crop's actual ET. To improve SWAT performances in runoff simulation in small basins, Kim (2010) improved the channel routing module of SWAT by developing a new channel routing mechanism. White (2010) changed the curve-number based SWAT into a new water-balance-SWAT, improving watershed runoff simulation in conditions such as monsoonal climates and areas dominated by variable source area hydrology. To address the special hydrological processes and crop yields in paddy rice areas, Xie (2011) develop the SWAT model by incorporating new processes for irrigation and drainage.

2.3 HYDROLOGIC MODEL CALIBRATION

Whether lumped or distributed, every hydrologic model contains parameters, quantities that control the response of the watershed or spatial segment to external forcing (i.e., precipitation and other climatic processes). Some parameter values cannot be determined from physical measurement and must be estimated in the process of model calibration. Calibration can be broadly defined as finding the set of parameter values that results in the best match between model generated and observed values.

Model calibration is a very complex process. The complexity includes the limitations of the models, limitations of the input and output data, imperfect knowledge of the basin characteristics, mathematical structure of the models and limitations in our ability to express quantitatively our preference how best to fit the models to data.

These limitations bring two problems to model calibration. First is that how to decide whether one set of parameter values is preferred over another set. In the case of automatic calibration this means to specify an objective function or a set of objective functions. Second is that how to select one set among all preferred sets to best apply the model. (Duan, 2002)

2.3.1 Optimization algorithm

When calibrating a model, a particular set of parameters needs to be obtained to best satisfy the model's requirement. This model requirement is usually expressed in mathematical equations, which are function of the parameter set

values. Then the problem of obtaining the best parameter set for the model are transformed into obtaining the parameter set that minimize the objective function. The minimizing procedure of the objective function is optimization.

Optimization methods are generally divided into two types according to their optimization results: local search and global search methods. Local search methods are earlier methods which can find only the local optima while global search methods are more capable of finding a global optimal.

Local-search optimization methods were first employed in watershed model calibrations. The two broad categories of local- search methods are direct type and gradient type. Direct type methods place a few limitations on the form of model equations, and require only that knowledge of the objective function values be available over the feasible parameter space. Gradient type methods require that model equations be continuous to second order, and that the knowledge of the objective function values as well as gradient be available.

Research found out that local-search methods are inherently incapable of finding the global optimal parameters. The methods cannot handle the presence of multiple regions of attraction, multi-local optima, discontinuous derivatives, insensitivity and parameter interdependency, and other problems encountered in watershed model calibration.

To deal with all problems inherited in local-search methods, global-search methods have been developed. Many global-search methods were developed since 1950s and 1960s, such as Generalized Gridding Methods, Interval Methods, Trajectory Methods, and Penalty Methods. Three commonly used

global optimization methods in watershed modeling are: Simulated Annealing, Generic Algorithm and Shuffled Complex Evolution. (Duan, 2002)

2.3.2 Automatic calibration of hydrologic models

Hydrologic models are well known for their large amount of parameters. Manually adjusting these parameter values depends on the subjective assessment of the modeler and is time consuming as well. Therefore, analysts seek automatic parameter-estimation methods.

Eckhardt (2001) developed an auto-calibration version of SWAT, which employed the Shuffled Complex Evolution Method for optimization.

Muleta (2004) described an automatic approach for calibrating daily stream flow and daily sediment concentration values estimated by SWAT. The automatic calibration approach automatically calibrates the model, carries out global parameter sensitivity analysis and generalized likelihood uncertainty estimation.

Bekele and Nicklow (2006) carried out a research on automatic calibration of SWAT model using a non-dominated sorting genetic algorithm II (NSGA-II). Confesor (2007) also used NSGA-II to auto-calibrate the SWAT model.

Kannan (2007) developed an automated procedure, which is developed to calibrate spatial variation of annual average runoff components for each USGS eight-digit watershed of the United States. It uses nine parameters to calibrate water yield, surface runoff and sub-surface flow respectively.

Jae Heon Cho and Sung Ryong Ha (2010) developed an automatic calibration model for QUAL2K by introducing an influence coefficient algorithm and a genetic algorithm (GA). Their method POMIG showed good calibration results.

Yongtai Huang and Lei Liu (2010) combined a hybrid genetic algorithm HGA and a neural network NN model as a new HGA-NN approach, which can be used for multi-objective calibration of surface water quality models CE-QUAL-W2.

2.4 INTRODUCTION OF PEST

2.4.1 PEST history

PEST (acronym for Parameter ESTimation) is a nonlinear parameter estimation package. The purpose of PEST is to assist in data interpretation, model calibration and predictive analysis, where model parameters need to be adjusted until model-generated numbers fit a set of observations as closely as possible, provided certain continuity conditions are met. PEST will adjust model parameters until the fit between model outputs and laboratory or field observations are optimized in the weighted least squares sense. The PEST software exists independently of any particular model, yet can be used to estimate parameters, and carry out various predictive analysis tasks, for a wide range of model types (Doherty, 2005).

Essentially, PEST automates the process of running a model repeatedly with parameter perturbations for sensitivity analysis or optimization.

2.4.2 The PEST optimization method

In PEST, the objective function is the weighted- squared-residual for all observations. The minimizing of the objective function can be expressed as:

$$\frac{\partial OF}{\partial p_i} = 0 \quad \text{Eq. 2.2}$$

where OF is the objective function, p_i is the i^{th} parameter value.

For nonlinear models, the derivatives of the objective function with respect to each parameter are estimated with a linear approximation, using Taylor's theorem and applying small deviations of the parameters (Δp_i). The above equation can be estimated as:

$$\frac{\Delta OF}{\Delta p_i} = 0 \quad \text{Eq. 2.3}$$

Each iteration begins with an initial set of parameter values, and the corresponding value of the objective function value (OF). The i^{th} parameter value is modified from p_i to $p_i + \Delta p_i$ while all other parameters are kept unchanged. The model is executed and the objective function is recalculated (OF_i). If the value of OF_i is less than the value of OF , the i^{th} parameter value would be updated to $p_i + \Delta p_i$, where Δp_i can be positive or negative.

Using the same procedure, the $(i+1)^{\text{th}}$ parameter value is modified from p_{i+1} to $p_{i+1} + \Delta p_{i+1}$ while all other parameters are kept unchanged. The objective function is recalculated (OF_{i+1}). If the value of OF_{i+1} is less than the value of OF_i , the i^{th} parameter value would be updated to $p_{i+1} + \Delta p_{i+1}$.

In each iteration, a factor for parameter moving step λ is used to make value change for all parameters. The Marquardt-Levenberg Method is used to determine the λ value (Marquardt 1963).

The iteration stops when all the parameters have been perturbed. The next iteration uses the final parameter values from the previous iteration as initial estimates and continues updating the parameters in the above procedure. When PEST's termination criteria (section 2.4.4) are met, the optimization process stops and the best parameter set is obtained.

2.4.3 Operations of PEST

Note: This section is quoted and summarized from PEST Manual (Doherty, 2004)

PEST must be provided with three types of input files that contain the data needed to effectively take control of a particular model:

- template files, one for each model input file which PEST must write before a model run,
- instruction files, one for each model output file which PEST must read after a model run,
- a PEST control file, which supplies PEST with the names of all template and instruction files together with the model input/output files to which they pertain. It also provides PEST with the model name, parameter initial estimates, field or laboratory measurements to which model outcomes must

be matched, prior parameter information, and a number of PEST variables that control the implementation of the optimization method.

Of the masses of data of all types that may reside in a model's input files, those numbers must be identified which PEST is free to alter and optimize. This process is carried out using input file "templates". To construct a template file, the analyst starts with a model input file and replaces each space occupied by a parameter with a text string (set of characters) that simultaneously identifies the parameter and defines its location and length in the input file. Each time PEST runs the model, it creates a new version of the input file, replacing the text string with a numerical value of the parameter.

Those numbers in a model output file for which must be matched to actual values will be referred to simply as "modeled observations". In order to peruse a model output file and read the modeled observation values, PEST must be provided with a set of instructions. For each model output file that must be read, PEST requires an instruction file that details how to find the modeled observations from that file. The analyst must prepare the template and instruction files using a text editor. The control file can also be prepared with a text editor, or using the program PESTGEN.

When the model interface is complete, PEST's role is to adjust the parameter values to minimize the weighted sum of squared differences between model-generated observation values and those actually measured in the laboratory or field; this sum of weighted, squared, model-to-measurement discrepancies is known as the "objective function" (as described in Section 2.4.2). (Doherty, 2004)

2.4.4 Termination criteria

PEST uses “a number of different criteria to determine when to halt this iterative process. There are two types of indicators that either the objective function is at, or very close to, its minimum, or that further PEST execution is unlikely to get it there” (Doherty, 2004).

The first type of criteria is the behavior of the objective function itself. If it has been reduced very little or not at all over a number of successive iterations, PEST would cease execution. The exact criteria that determine this type of termination are set through PEST input variables PHIRESTP, NPHISTP, and NPHINORED.

The second type of indicator is the behavior of the adjustable parameters. In this circumstance, the indicators convergence to the objective function minimum, or further iterations are unlikely to achieve the objective function minimum. If successive iterations are effecting little change in parameter values, there is probably little to gain in continuing with PEST execution. The exact criterion is the input variables RELPARSTP and NRELPAR. (More details available in the PEST Manual, [Doherty, 2005]).

2.4.5 Hydrologic applications of PEST

PEST has been widely applied in hydrology. Many researchers have used PEST for parameter estimation and sensitivity analysis in soil and water related models.

The modeling package Annualized Agricultural Nonpoint Source Model (AnnAGNPS) was applied to predict the export of nitrogen and phosphorus from Currency Creek, a small experimental catchment within the Hawkesbury–Nepean drainage basin of the Sydney Region. PEST was applied for sensitivity testing to determine and assess the relative importance of the key parameters of the model (Baginska et al., 2002)

Zyvoloski (2003) presented several different conceptual models of the Large Hydraulic Gradient (LHG) region north of Yucca Mountain and describes the impact of those models on groundwater flow near the potential high-level repository site. The numerical models are calibrated by matching available water level measurements using PEST, along with more informal comparisons of the model to hydrologic and geochemical information.

Immerzeel (2007) coupled PEST with SWAT in calibrating a model in the Krishna basin in southern India. Wang and Melesse (2005) used PEST to adjust their SWAT model. They further modified the PEST-generated parameter values and determined that SWAT performs well in snowmelt hydrology.

Islama and Wallender (2005) auto-calibrated a MIKE SHE model with PEST to investigate the effects of winter cover cropping practices on water availability.

In order to link the Army Remote Moisture System (ARMS) with the Land Information System (LIS), PEST was integrated into the process to optimize soil porosity and saturated hydraulic conductivity (K_{sat}), using remotely sensed measurements, in order to provide a more accurate estimate of the soil moisture (Tischler and Garcia, 2006).

Iskra and Droste (2007) conducted a study on the effects of three automatic optimization techniques, Levenberg-Marquardt Method (PEST), Random Search Method and Shuffled Complex Evolution Method, on calibrating an HSPF model. They found that SCE performed best, and that PEST can perform as well as SCE if the variables are properly adjusted, initial guess is good and insensitive parameters are eliminated from the optimization process.

In one study, PEST was used to calibrate the Noah land surface model run at very high spatial resolution across the Walnut Gulch Experimental Watershed. The results demonstrate the potential to gain physically meaningful soil information using simple parameter estimation with few but appropriately timed remote sensing retrievals (Santanello, 2007).

PEST was also used to calibrate a MODFLOW2000 (groundwater) model at Lake Tegel, Berlin, Germany, demonstrating a leakage concept which is based on the assumption of the influence of an unsaturated zone on clogging processes (Wiese, 2008).

In another study, methods of global analysis (Latin hypercube sampling, LHS) and gradient-based optimization (PEST) were explored to calibrate soil hydraulic parameters in the Root Zone Water Quality Model (RZWQM2). Errors in simulated soil water content were reduced by using LHS to initialize and constrain the PEST parameter space, which also stabilized the cross-validation results (Fang, 2009).

CHAPTER THREE

THE NEW GROUNDWATER ALGORITHM

3.1 INTRODUCTION OF THE HYDROGRAPH

By definition, a hydrograph is a plot of the variation of discharge with respect to time. It can also be the variation of stage or other water property with respect to time. Discharge is the volume of water flowing past a location per unit time (usually in cubic feet per second [cfs]). (NOAA, 2011)

In surface water hydrology, a hydrograph is a time record of the discharge of a stream, river, or watershed outlet. Rainfall is typically the main input to a watershed and the streamflow is often considered the output of the watershed; a hydrograph is a representation of how a watershed responds to rainfall. Hydrographs are used in hydrology and water resources planning.

3.2 INTRODUCTION OF BASEFLOW SEPARATION

The runoff hydrograph is conceptually separated into two parts: direct runoff and baseflow. Direct runoff is the storm runoff that results from rainfall excess. Baseflow is runoff that has resulted from an accumulation of water in the watershed from previous precipitation, which infiltrates in to the soil, percolates to the groundwater table, and moves laterally to reappear as surface runoff. Baseflow would appear as streamflow even if the rain for the current storm event had not occurred. (McCuen, 2005)

Hydrograph separation is often necessary in flood analysis, because the quick response of direct runoff is important in designing flood control structures.

Separation of a hydrograph is often performed on the basis of analytical procedures rather than physical processes.

To separate baseflow, three features need to be identified: the start and end of surface runoff and the shape of the baseflow hydrograph between these two points. The starting point of direct runoff (t_s) is generally defined as the lowest point of discharge rate before a storm event (rainfall excess) occurs. The ending point of surface runoff (t_e) and the baseflow hydrograph shape vary in the different separation methods.

The most common separation methods include: constant-discharge method, constant-slope method and concave method (McCuen, 2005):

3.2.1 Constant-Discharge Method

The line separating baseflow and direct runoff begins at the point of the lowest discharge rate at the start of flood runoff and extends at a constant discharge rate until it intersects the recession limb of the hydrograph.

This simple method requires no calculations, but it is not always applicable. There may not be an intersection on the recession limb. In such cases, direct runoff would never end, which is unrealistic.

3.2.2 Constant-Slope Method

The starting point of direct runoff is the point of the lowest discharge rate. The ending point is identified by the inflection point on the hydrograph recession (t_i). The inflection point is the point where the hydrograph goes from being concave

to convex. Another way to find the inflection is using an empirical formula. The equation (McCuen, 2005) below has been proposed for very large watersheds,

$$N = A^{0.2} \qquad \text{Eq. 3.1}$$

in which N is the number of days from the time to peak (t_p) of the measured runoff hydrograph to the end of direct runoff, and A is the drainage area in square miles. If t_r is calculated from the empirical equation above, then $t_r = t_p + N$ (Figure 3.1).

A straight line connecting these two points separates baseflow (the lower part) from direct runoff (the upper part). It should be noted that the selection of inflection point is generally determined by inspection of the runoff hydrograph.

3.2.3 Concave Method

The starting and ending points of direct runoff are the same as the Constant-Slope Method. However, for the concave method, baseflow continues to decrease (in constant slope equal to the slope before the storm event) until the time of the peak discharge of the storm hydrograph. At that time, the separation line becomes a straight line between that point and the inflection point on the recession.

Although this method requires more calculation than the other two methods, it is a more realistic representation of the physical processes that control flow during storm events.

The Constant Slope and Concave Methods both reflect the physical reality that subsurface flow – as well as direct surface runoff – is generated during an event, reaching a peak later than the surface flow peak. The three methods for baseflow separation are summarized in Figure 3.1.

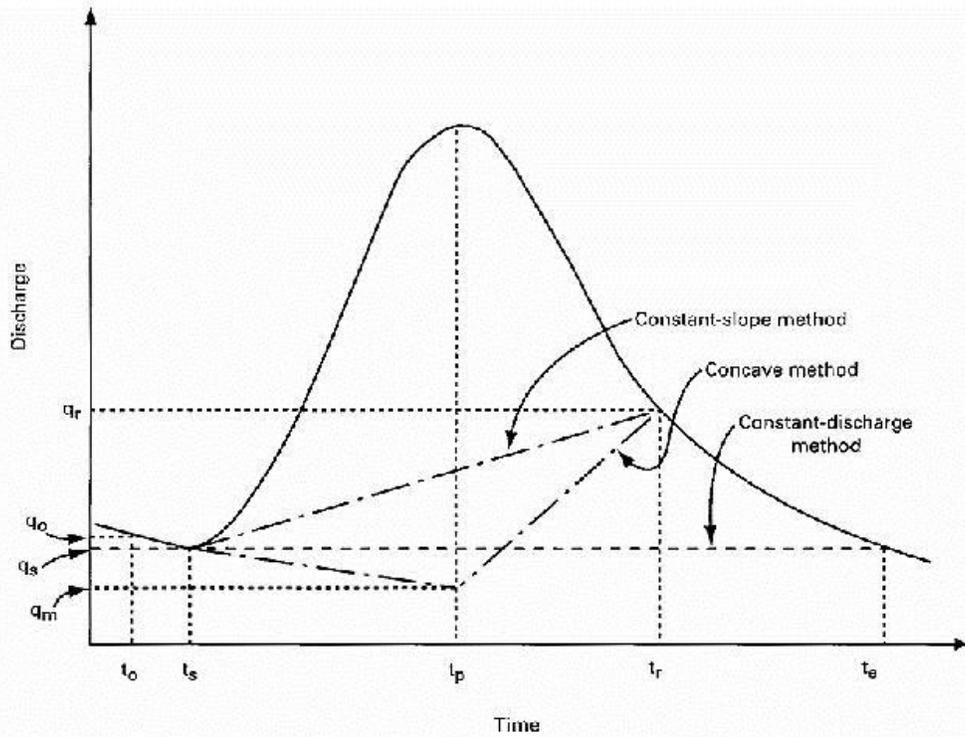


Figure 3.1 Baseflow Separation Methods (McCuen, 2005)

3.3 SWAT BASEFLOW ALGORITHM

A process-based hydrologic model, such as SWAT, synthesizes the runoff hydrograph by representing the surface and subsurface processes that contribute to event response. The model calculates the flow contributions separately using conservation of mass for the surface and subsurface. In SWAT, the subsurface is divided into a shallow aquifer, which provides baseflow to

streams, and a deep aquifer, which does not interact with streams. (Neitsch, 2005)

The water balance for a shallow aquifer can be expressed as

$$aq_{sh,i} = aq_{sh,i-1} + w_{recharg,sh} - Q_{gw} - w_{relep} - w_{pump,sh} \quad Eq. 3.2$$

where $aq_{sh,i}$ is the amount of water stored in the shallow aquifer on day i ,

$aq_{sh,i-1}$ is the amount of water stored in the shallow aquifer on day $i - 1$,

$w_{recharg,sh}$ is the water recharge into the shallow aquifer on day i ,

Q_{gw} is the groundwater flow into the streams on day i ,

w_{relep} is the water that re-evaporate into the air on day i ,

$w_{pump,sh}$ is the pumped from shallow aquifer on day i .

Assuming there is no pumping, no re-evaporation, and no percolation into deep aquifer, the water balance can be simplified as:

$$aq_{sh,i} - aq_{sh,i-1} = w_{recharg,sh} - Q_{gw} \quad Eq. 3.3$$

The steady-state recharge to a river (Hooghoudt, 1940) is

$$Q_{gw} = \frac{8000K}{L^2} \cdot h_{wtbl} \quad Eq. 3.4$$

where K is the hydraulic conductivity of the aquifer,

L is the distance from the ridge for the groundwater basin to the main channel,

h_{wtbl} is the water table heights of the aquifer,

The non-steady state recharge (non-steady fluctuation of the water table) can be expressed as

$$\frac{dh_{wtbl}}{dt} = \frac{w_{rcharg,sh} - Q_{gw}}{800\mu} \quad Eq. 3.5$$

where μ is the specific yield of the aquifer.

The original version of SWAT assumes that the groundwater flow is directly proportional to the groundwater storage (which can be presented as water table height). This is known as the linear-reservoir assumption. Using Equation 3.4 and 3.5, gives

$$\begin{aligned} \frac{dQ_{gw}}{dt} &= \frac{8000K}{L^2} \cdot \frac{w_{rcharg,sh} - Q_{gw}}{800\mu} = 10 \frac{K}{L^2\mu} (w_{rcharg,sh} - Q_{gw}) \\ &= \alpha_{gw} (w_{rcharg,sh} - Q_{gw}) \end{aligned} \quad Eq. 3.6$$

where α_{gw} is the groundwater recession constant.

Solving Equation 3.6, Q_{gw} is

$$Q_{gw,i} = Q_{gw,i-1} \cdot e^{-\alpha_{gw}t} + w_{rcharg,sh}(1 - e^{-\alpha_{gw}t}) \quad Eq. 3.7$$

where i is the time index. Note that only when the storage in shallow aquifer exceeds one particular value, generally defined by modelers according to historical data or experience, can groundwater reach the river ($Q_{gw,i} > 0$). In SWAT, parameter GWMIN is used to represent the threshold depth of water in the shallow aquifer required for return flow to occur.

When no recharge is occurring, the solution simplifies to

$$Q_t = Q_0 e^{-t/k} \quad \text{Eq. 3.8}$$

where Q_t is the discharge at time t ,

Q_0 the initial discharge,

k the recession constant which can be considered to represent average response time in storage.

In other words, the hydrograph for pure baseflow from a linear groundwater reservoir follows an exponential decay curve.

Ever since Maillet (1905), the exponential function of Eq. 3.8 has been widely used to describe the groundwater baseflow recession. The exponential function implies that the groundwater aquifer behaves like a single linear reservoir with storage that is linearly proportional to outflow:

$$\frac{dS}{dt} = -Q_t \quad \text{Eq. 3.9}$$

$$S = kQ_t \quad \text{Eq. 3.10}$$

The SWAT modeling environment, using this algebra, assumes a linear-reservoir groundwater baseflow as explained earlier.

3.4 THE NEW BASEFLOW ALGORITHM

Observation have shown that the parameter k fitted to different discharge ranges of the recession curves in actual rivers does not remain a constant but increases systematically with the decrease of streamflow (Wittenberg, 1994; Moore, 1997), which is a strong indication of nonlinearity.

Moreover, the linear-reservoir baseflow model is inappropriate in our study because of the special geographic formation of the area. The area in our study,

the Shenandoah Valley is famous for its Karst formation. Aquifers in this area consist of various sinkholes and hydraulically communicating pore and fissure systems. The macro pores in soil formation greatly affect the uniformity of aquifer, which is a key pre-requisite for the linear assumption. Studies by ICPRB of baseflow from various regions in the Potomac River Basin have also indicated that the exponential decay is not appropriate.

Therefore, a non-linear algorithm is investigated in this study. To allow for nonlinearity, the relationship between subsurface flow and shallow aquifer storage is generalized by adding an exponent b as follows:

$$S = kQ^b \quad \text{Eq. 3.11}$$

In SWAT, baseflow is allowed to enter the reach only if the amount of water stored in the shallow aquifer exceeds a threshold value S_{min} (this value is specified by the user). Therefore, the baseflow would only occur when $S > S_{min}$, and the new algorithm is

$$S - S_{min} = kQ^b \quad \text{Eq. 3.12}$$

$$Q = \left(\frac{S - S_{min}}{k} \right)^{1/b} = \left(\frac{S - S_{min}}{\alpha} \right)^{1/\beta} \quad \text{Eq. 3.13}$$

where S is shallow aquifer storage [L]

S_{min} is the minimum storage for GW flow [L]

α is a scale parameter [$T^b L^{3(1-\beta)}$]

β is a coefficient [dimensionless]

If $\beta = 1$, the new model becomes the same as the linear model equation 3.8.

This new algorithm required editing the groundwater module in the SWAT code and recompiling the entire program. The ICPRB team performed this process to produce the modified version of SWAT, called iSWAT. The change also required a small modification to the groundwater parameter input files. An example of the new groundwater parameter input file is shown below. The new Beta Parameter is listed in the last row. Besides the additional parameter, GWMIN in the new input file has a different meaning than the original SWAT version. In the original SWAT, GWMIN represents the threshold depth of water in the shallow aquifer required for baseflow to occur. In the modified version, GWMIN represents the threshold storage required for baseflow to occur.

```
.gw file Subbasin:6 HRU:18 Luse:HAY Soil: VA066 Slope: 10-9999 7/31/2009 12:00:00 AM ARCGIS-SWAT interface MAVZ
  0.5000 | SHALLST : Initial depth of water in the shallow aquifer [mm]
1000.0000 | DEEPST : Initial depth of water in the deep aquifer [mm]
 31.0000 | GW_DELAY : Groundwater delay [days]
  0.0480 | ALPHA_BF : BAseflow alpha factor [days]
  0.0000 | GWMIN : Threshold depth of water in the shallow aquifer required for return flow to occur [mm]
  0.0200 | GW_REVAP : Groundwater "revap" coefficient
  1.0000 | REVAPMN: Threshold depth of water in the shallow aquifer for "revap" to occur [mm]
  0.0500 | RCHRG_DP : Deep aquifer percolation fraction
  1.0000 | GWHT : Initial groundwater height [m]
  0.0030 | GW_SPYLD : Specific yield of the shallow aquifer [m3/m3]
  0.0000 | SHALLST_N : Initial concentration of nitrate in shallow aquifer [mg N/l]
  0.0000 | GWSOLP : Concentration of soluble phosphorus in groundwater contribution to streamflow from subbasin [mg P/l]
  0.0000 | HLIFE_NGW : Ha;f-life of nitrate in the shallow aquifer [days]
  1.0000 | BETA_BF : Baseflow "beta" factor for ICPRB version of SWAT
```

Figure 3.2 iSWAT input file with modified groundwater parameter

CHAPTER FOUR

MODEL SETUP

4.1 WATERSHED DELINEATION

To set up a SWAT model, watershed segmentation is the first step. A proper division and classification of the study area in size and land use is essential for hydrologic model. In this Shenandoah Valley Model, watershed division is carried out in three successive levels.

4.1.1 Level one: Hydrologic Unit Code

The basic spatial segmentation follows the USGS 8-digit Hydrologic Unit Codes (HUC) (USGS, 2011). The United States is divided and sub-divided into successively smaller hydrologic units which are classified into four levels: regions, sub-regions, accounting units, and cataloging units. Each hydrologic unit is identified by a unique hydrologic unit code (HUC) consisting of two to eight digits based on the four levels of classification in the hydrologic unit system.

The first level of classification divides the Nation into 21 major geographic areas, or regions. These geographic areas contain either the drainage area of a major river, or the combined drainage areas of a series of rivers (Figure 4.1). The second level of classification divides the 21 regions into 221 subregions. A subregion includes the area drained by a river system, a reach of a river and its tributaries in that reach, a closed basin(s), or a group of streams forming a coastal drainage area. The third level of classification subdivides many of the

subregions into accounting units. These 378 hydrologic accounting units are nested within the subregions, or in some cases, are equivalent to the subregion. The fourth level of classification is the cataloging unit, the smallest element in the hierarchy of hydrologic units. A cataloging unit is a geographic area representing part of all of a surface drainage basin, a combination of drainage basins, or a distinct hydrologic feature. These units subdivide the subregions and accounting units into smaller areas. There are 2264 Cataloging Units in the Nation. Cataloging Units sometimes are called "watersheds."

The Mid-Atlantic Region is numbered 02 (first level); the Potomac River Basin is numbered 07, giving the second-level regional code 0207; region 0207 includes only one accounting number (00); therefore the entire region has third-level code 020700. Each smaller watershed within the Potomac Region is numbered with a 2-digit ID for a total of eight digits. The Potomac Basin contains 11 eight-digit cataloging units (Figure 4.2).

This work focuses on the three watersheds: South Fork Shenandoah Watershed (02070005), the North Fork Shenandoah Watershed (02070006), and the Shenandoah (Lower Shenandoah) Watershed (02070007).

4.1.2 Level two: Subwatersheds

For the SWAT model development, each HUC is further subdivided into subwatersheds on the basis of the topography (via Digital Elevation Model) and the stream network. The subwatershed is the fundamental spatial unit in the

SWAT environment. Hydrologic routing occurs within and between subwatersheds and their corresponding stream reaches.



Figure 4.1 United States HUCs (USGS, 2011)

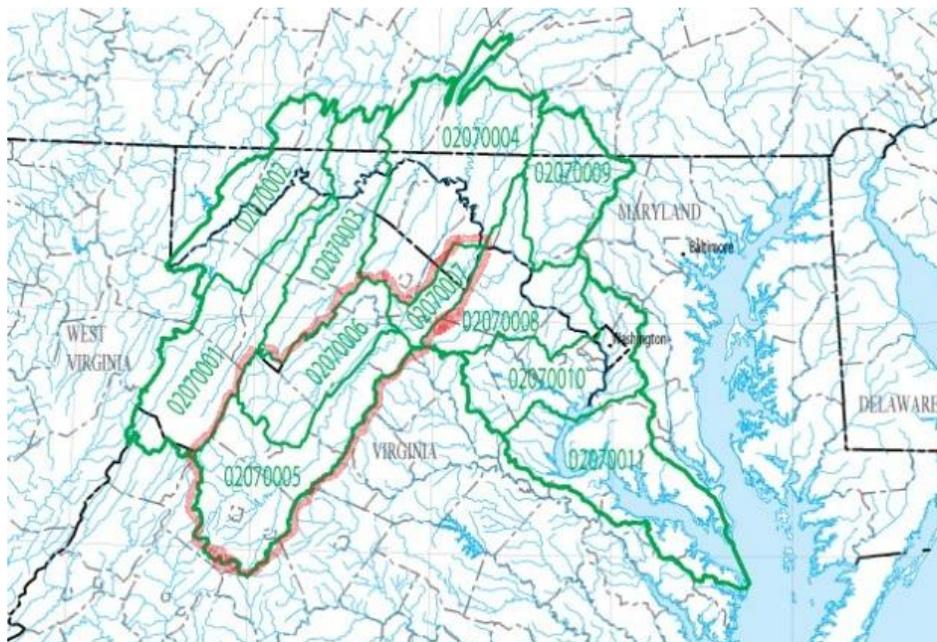


Figure 4.2 Potomac Basin (USGS, 2011): Red curve outlines the study area.

Eight-digit codes indicate the national cataloging units (HUCs)

A total of 28 subwatersheds are studied in this work. The South Fork Shenandoah Watershed (HUC 02070005) is further divided into twelve subwatersheds. They are numbered as subbasin 0501-5012. The North Fork Shenandoah Watershed (HUC 02070006) is further divided into ten subwatersheds, numbered from 0601 to 0610. The Lower Shenandoah Watershed (HUC 02070007) is divided into six subwatersheds, numbered from 0701 to 0706. Subwatershed outlets are defined at USGS gauges and other locations as defined by the stream network (Figure 4.3).

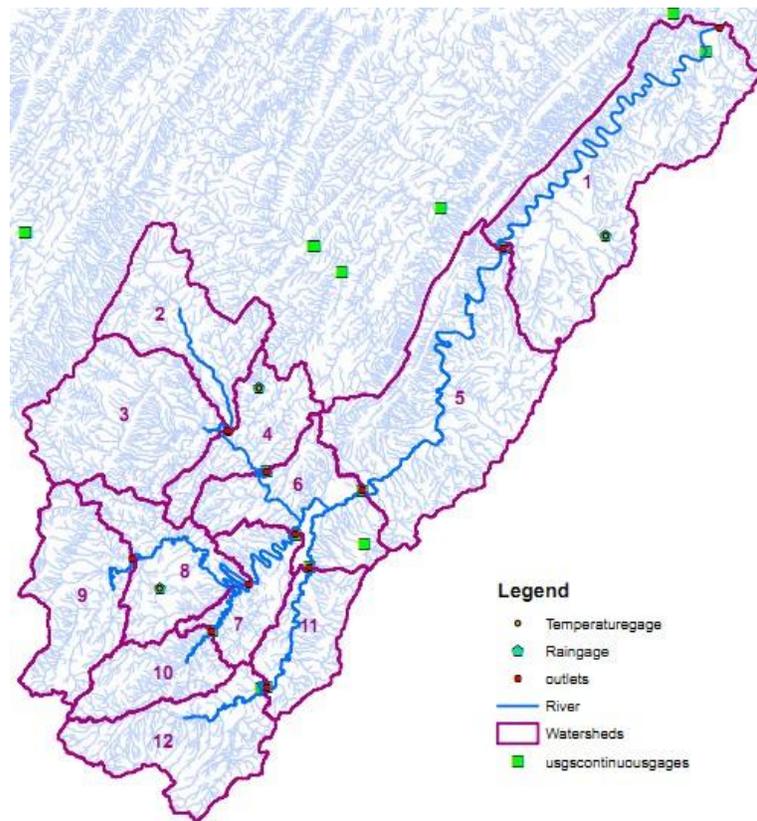


Figure 4.3 Subbasins within South Fork Shenandoah (0705)

4.1.3 Level three: Hydrologic Response Units

Subwatersheds are further divided into Hydrologic Response Units (HRUs) on the basis of land use, soil, and slope. An HRU is a Hydrologic Response Unit, the smallest homogeneous area in the model. Unlike the subwatersheds, the HRUs are not spatially defined. All land with similar characteristics within the subwatershed is grouped into an HRU, whether or not these land areas are adjacent to each other. Each HRU is assumed to be homogeneous for each attribute such as soil type or vegetation density (USGS, 2010b).

If all possible combinations of soil types, land used and slope are modeled in the watershed, there would be a large number of very small HRUs. Therefore, a subjectively defined segmentation method was employed. The ArcSWAT interface was used to automate this grouping process.

This HRU analysis was carried out by the ICPRB team in a GIS environment using raster data: one layer for land use, one for soil, and one for slope. Land use and soil are categorical data. In this work, the team defined five land use classes: urban low-density, urban mid-density, urban high-density, forest and hay. For soil types, the team defined 12 classes. The detailed soil type classification is provided in Table 4.1. Note that VA069 and WV010, VA005 and WV119 are of the same soil type. Different notation is due to different naming methods by the two states (Virginia and West Virginia). The team also defined two slope classes: less than; and greater /equal to 10% slope.

Table 4.1 Soil Descriptions and Classification in this SWAT Model (USDA-NRCS)

Soil Name	Soil ID(s) in the Model	Parent rock*	Parameter code for ESCO and SLSOIL	Parameter code for ALPHA_BF and Beta_BF
BERKS	VA066	shale, siltstone and fine grained sandstone	_va066	_sss
CARBO	VA002	limestone bedrock	_va002	_lim
EDGEMONT	WV114	quartzitic rocks	_wv114	_qua
FREDERICK	VA003	dolomitic limestone with interbeds of sandstone, siltstone, and shale	_va003	_lss
HAGERSTOWN	VA069, WV010	hard gray limestone	_va069	_lim
L Aidig	VA016	colluvium from sandstone, siltstone, and some shale... benches and foot slopes	_va016	_col
LILY	VA005, WV119	sandstone	_va005	_san
MOOMAW	VA004	alluvium derived from acid sandstone, quartzites, and shales	_va004	_col
MYERSVILLE	VA006	basic crystalline rocks, including greenstone	_va006	_cry
WEIKERT	VA001	interbedded gray and brown acid shale, siltstone, and fine-grained sandstone	_va001	_sss

In the ArcSWAT interface, the ICPRB team used a grouping rule of 20/10/0 for Land Use / Soil / Slope. This means that pixels of different land use may be grouped together as long as a minority land use does not exceed 20% of the resulting HRU, a minority soil does not exceed 10% of the HRU, and slope classes may not be mixed. The non-mixed procedure for slope was applied because slope is particularly important in the runoff generation process. The urban land uses were exempted from the grouping rule, which means that even if a subbasin has a very small fraction of low-density, medium-density, or high-

density developed land, a separate HRU was defined for each. The reasoning was that this would make it easier to conduct future experiments in changing the fractions of land uses within a subbasin. For the 28 subwatersheds, 489 HRUs are defined.

Examples of soil map, land slope map, and landuse map are shown in Figures 4.4, 4.5, and 4.6. These figures show the soil types, land slope (classified as <10% and ≥10%), and land use for Lower Shenandoah Watershed (02070007).

It is important to note that the HRUs are not spatially contiguous. They are grouped response units. The pixels making up a given HRU may be spread across the subbasin. Water is not routed between HRUs; rather, the unit HRU contribution is scaled by the area fraction of that HRU in the subwatershed (in this way, SWAT is similar to other watershed modeling environments such as HSPF).

4.2 INPUT FILES NEEDED FOR SWAT

SWAT requires precipitation and temperature data for each subbasin to simulate waterflow within and between subbasins.

Precipitation data are needed because it is the driving force for water cycle. In this iSWAT model, precipitation data is obtained from National Climate Data Center. Nine stations were chosen to provide precipitation data as input for ArcSWAT. A text input file shenall.pcp contains daily precipitation values from 1994 to 2006 listed in nine columns, one for each station. The stations are numbered from 1 to 9.

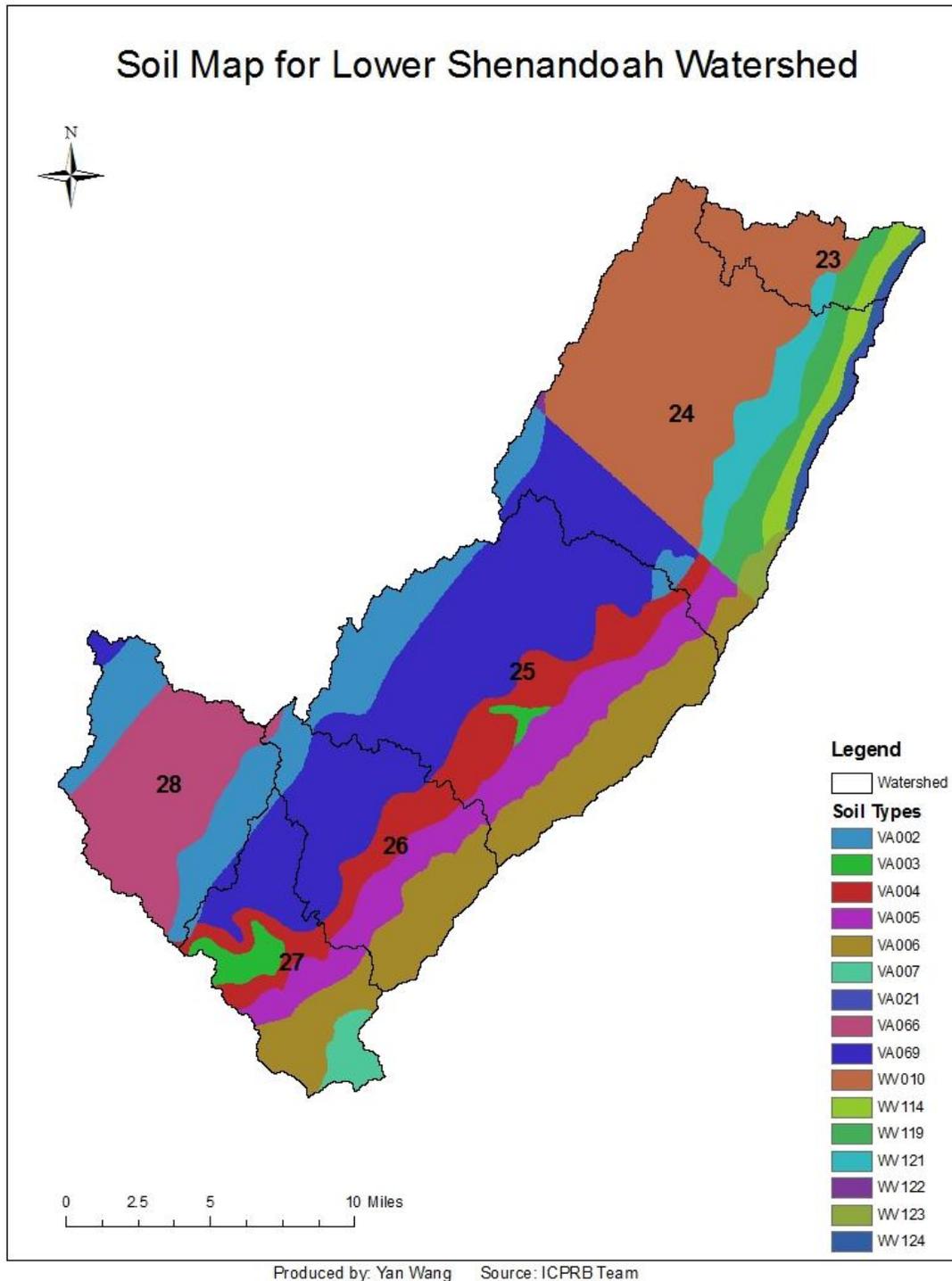


Figure 4.4 Soil Types in Lower Shenandoah. Soils are identified in Table 4.1

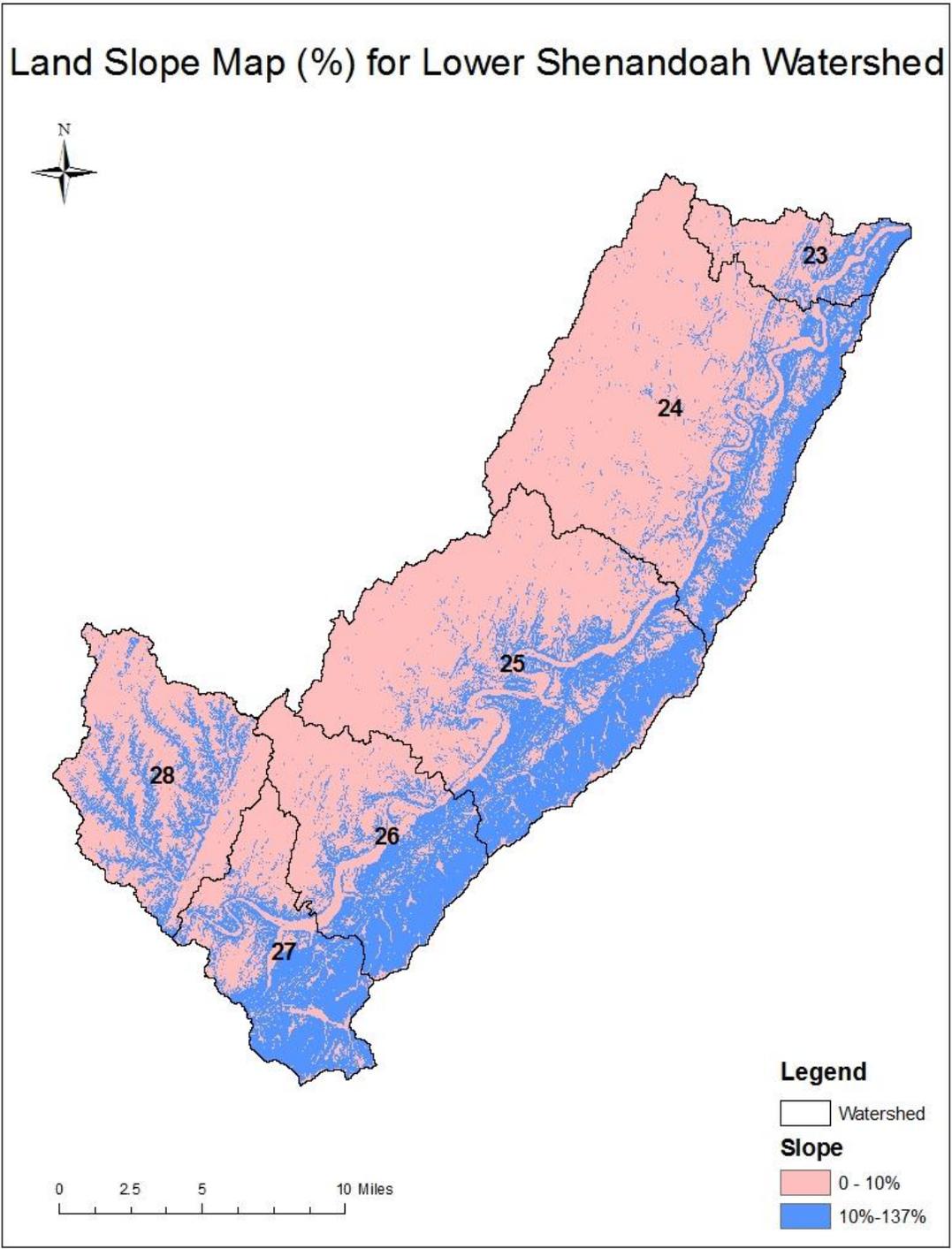


Figure 4.5 Land Slope in Lower Shenandoah

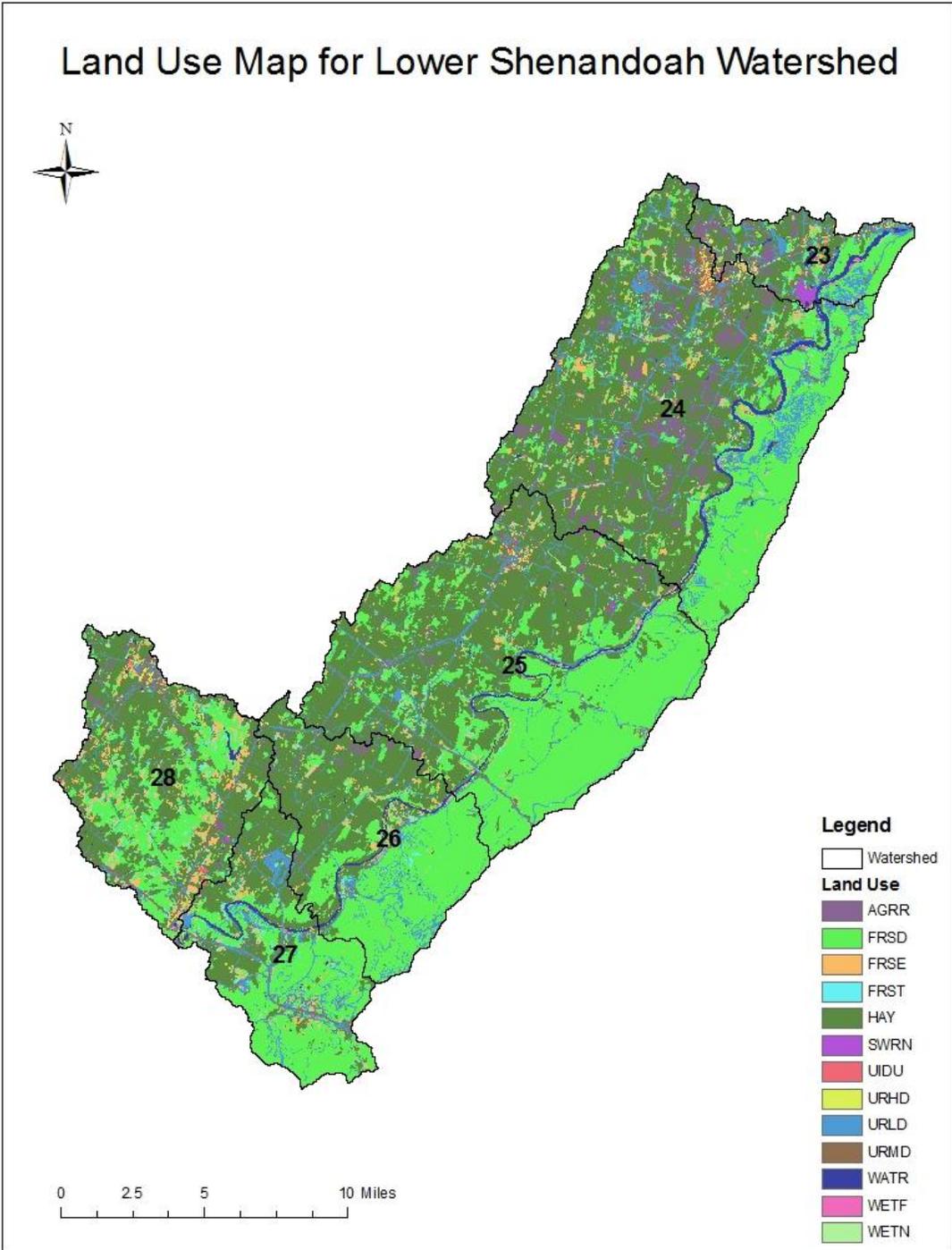


Figure 4.6 Land Use in Lower Shenandoah

Since precipitation is a subbasin level data input, all HRU share the same amount and type of precipitation (rainfall or snow). ArcSWAT assigns the nearest precipitation data (precipitation station) to each subbasin. In each .sub file, index of the precipitation station is called to identify which station's data would be used as SWAT input for this specific subbasin.

The precipitation station index in SWAT, Cooperative Station ID assigned by National Oceanic and Atmospheric Administration (NOAA), the name, and the location of each precipitation station are listed in Table 4.2. Also included are the subbasins assigned to each station.

Table 4.2 Precipitation Data Used in SWAT

ID(SWAT)	ID(NOAA)	Name	County	State	Subbasins included
1	442208	Dale Enterprise	Rockingham	VA	0501
2	442663	Edinburg	Shenandoah	VA	0502, 0503, 0504, 0607, 0609, 0610
3	443229	Front Royal	Warren	VA	0505, 0506, 0507, 0508, 0509, 0510, 0511, 0512
4	445096	Luray 5 E	Page	VA	0601
5	445851	MT Weather	Loudoun	VA	0602, 0704, 0705, 0706
6	448062	Stauton Water Treatment	Augusta	VA	0603, 0606
7	449263	Woodstock 2 NE	Shenandoah	VA	0605, 0608, 0604
8	467342	Ranson 4NW	Jefferson	WV	0701, 0702
9	469281	Wardensville RM Farm	Hardy	WV	0703

Temperature data are also needed because many hydrologic processes are closely related to temperature. SWAT classifies precipitation as rain or snow using the average daily temperature. Snowmelt is also controlled by the temperature of the air and snow pack. On the other hand, soil temperature

impacts water movement and the decay rate of residue in the soil. Plant growth and evapotranspiration are also strongly temperature dependent.

In this iSWAT Shenandoah model, daily temperature data were obtained from the National Climate Data Center. Six Stations were chosen to provide temperature data as input for ArcSWAT. In the temperature input file shenall.tmp, the daily minimum and maximum temperature values from 1970 to 2006 are listed in two columns for each station. A total of 12 columns are presented in the shenall.tmp file. The temperature stations are numbered from 1 to 6.

Temperature is also a subbasin level data input. All HRU within the subbasin share the same temperature value. ArcSWAT assigns the nearest temperature station for each subbasin. In each .sub file, the number of temperature station is called to identify which station data is to be used as SWAT input for this specific subbasin. SWAT adjusts temperature for elevation using the difference between station elevation and subbasin average elevation.

A weather generator is used in SWAT to detailed weather conditions (SWAT Manual 1.3) other than precipitation and temperature (cloud cover, wind speed, etc.). The model generates a set of weather data for each subbasin, consistent with the observed precipitation and temperature. The values for any one subbasin are generated independently and there is no spatial correlation of generated values between the different subbasins.

The temperature station index in SWAT, Cooperative Station ID assigned by NOAA, the name and the location of each temperature station are listed in Table 4.3. Also included are subbasins assigned to each station.

Table 4.3 Temperature Data Used in SWAT

ID(SWAT)	ID(NOAA)	Name	County	State	Subbasins included
1	442208	Dale Enterprise	Rockingham	VA	0501
2	442663	Edinburg	Shenandoah	VA	0502, 0503, 0504, 0505, 0506, 0607, 0609, 0610
3	443229	Front Royal	Warren	VA	0507, 0508, 0509, 0510, 0511, 0512
4	445096	Luray 5 E	Page	VA	0601, 0606
5	448062	Stauton Water Treatment	Augusta	VA	0602, 0701, 0702, 0703, 0704, 0705, 0706
6	449263	Woodstock 2 NE	Shenandoah	VA	0603, 0604, 0605, 0608

Other input files are as described in section 2.2.3. In this iSWAT model, there are 28 subwatersheds, and 489 HRU in total. Therefore, the input files consist of one of each watershed-level file, 28 of each subbasin-level file, and 489 of each HRU-level file.

The Shenandoah iSWAT model does not include wetland and reservoir. The model does not simulate nutrients, pesticides, and other water quality related variables.

4.3 INPUT FILES FOR PEST --- COUPLING OF PEST AND SWAT

As explained in section 2.4.3, PEST performs model calibration by running the model many times with perturbed parameter values, then calculating the objective function by comparing model predictions to observations. The analyst needs to inform PEST which parameters need modification, how to modify the input files, and what information to extract from the model output files.

4.3.1 Selection of SWAT parameters for calibration

The first step in setting up PEST is to identify the SWAT parameters that need to be estimated in the calibration process.

The critical parameters in the Shenandoah model are water-quantity-related parameters. These parameters include evapotranspiration variables, soil character variables and roughness coefficients. A more detailed description of the parameters is listed in Table 4.4.

Each HRU input file allows specification of the HRU-level parameters. In principle, it would be possible to estimate 489 values of each, for example the soil evaporation efficiency ESCO or the plant uptake adjustment EPCO. The ICPRB team's philosophy for model calibration was to avoid such a large number of free parameters by associating these properties with soil type or plant type, as appropriate. Each of the 489 HRUs that has a given soil type is assigned the same value of ESCO; each HRU that has a given plant type is assigned the same value of EPCO. In addition to significantly reducing the dimension of parameter space, it was hoped that this approach would lend some physical rationality to the parameters.

Soil parameters

The names/IDs for soils are assigned by state. The same soil type can have different IDs in different states. Therefore, the same soil with different names is assigned one name as is shown in Table 4.1. For example, HAGERSTOWN soil is "VA069" in Virginia and "WV010" in West Virginia. The parameters ESCO and

SL_SOIL for HAGERSTOWN in both states are assigned the “va069” ID in the PEST routine. Therefore, although the Shenandoah watershed model has 489 HRUs, only 10 ESCO and SLSOIL parameters are used.

Plant parameters

The parameters EPCO and CANMX are set according to whether the HRU vegetation is crop or forest. Forest values are used for the urban land use HRUs. (The fact that urban land contains fewer trees than forest land is reflected in a canopy cover parameter that is prescribed, not adjustable.)

Groundwater parameters

The groundwater flow parameters are assigned on the basis of underlying geology, as inferred from the parent rock types associated with the various soil series (Table 4.1). Similar parent rock types were grouped to give seven sets of the three groundwater parameters for the Shenandoah model. That is, each of 489 HRUs was assigned one of seven parameter sets (ALPHA_BF, BETA_BF, and GW_DELAY). The SWAT environment tracks a groundwater storage model state on the HRU level. Model output must be checked to confirm that HRUs within the same subbasin have consistent trajectories of this model state variable, because the subbasin, not the HRU, is the spatial entity.

Channel roughness parameters

Channel roughness parameters (Manning’s n) were grouped on the basis of geology, on the assumption that the type of rock and soil that a stream flows through are the major controls on its roughness. The tributary channel roughness parameter was assigned on a subbasin basis, according to the dominant geologic group in the subbasin. The main channel roughness was assigned on a subbasin basis according to the geologic group associated with the soil type(s) through which the main channel flows, ascertained by visual inspection of the soil maps.

Table 4.4 Adjustable Parameters in iSWAT-PEST

In HRU files	ESCO	Adjustment factor for evaporation from soil	Vary by soil type
	EPCO	Adjustment factor for plant uptake of water by evapotranspiration	two values – crop and forest
	SL_SOIL	Subsurface flow length (interflow)	Vary by soil type
	CANMX	Maximum canopy interception	two values – crop and forest
In GW files	GW_DELAY	Time lag for appearance of groundwater flow in stream	Assigned on the basis of parent geology as inferred from soil type
	ALPHA_BF	Coefficient in groundwater recession	
	BETA_BF	Exponent in groundwater recession	
In BASINS file	SURLAG	Surface runoff lag coefficient	Applies to entire model domain
In SUB files	CH_N1	Manning’s “n” for the tributary channels	Vary by dominant geology of subbasin
In RTE files	CH_N2	Manning’s “n” for the main channel	Vary by geology corresponding to main channel

Surface Lag parameter

This is a basin scale parameter and can only be finally set when the entire Potomac basin model is calibrated. It was specified on a 3-HUC scale for the Shenandoah model.

4.3.2 Preparing PEST input files

As discussed in section 2.4.2, PEST template files (.ptf), instruction files (.pif) and control file (.pst) are required to run PEST. The template files allow PEST to perturb the selected parameters; the instruction files dictate how PEST extracts simulated values from model output; and the control file provides overall information for the calibration.

To construct a template file, the analyst starts with a model input file that contains parameters to be adjusted in calibration, and replaces each space occupied by an adjustable parameter with a set of characters that both identify the parameter and define its width in the input file. The parameter identification text is bracketed by a specific character (in this work '#' is used). The text "ptf@" is added in the first line of the text file before the main body. Finally, the file extension is changed into .ptf to identify the files as a PEST Template File.

SWAT model outputs needed for PEST analysis are flow discharge of each reach within the three subwatersheds. The information is included in the output.rch file. PEST instruction files direct the PEST software to the output files. Instruction files tell PEST which generated data should be used to compare with the observations. The number of instruction files is determined by the number of observation groups. The Shenandoah model has 15 observation groups (data from 15 gaging stations); therefore, 15 instruction files are needed.

In the PEST control file, an initial estimate is assigned to each parameter. Also required are the upper and lower bound of the parameter. In the control file, parameters may be identified as one of three types: "fixed" parameters remain

unchanged during iterations; “linked” parameters are adjusted in proportion to each other; otherwise (“none”), PEST is free to vary the parameter within its allowed range to improve the objective function.

Also, in the control file, each reach (gauged station) is given a weight for its contribution to the model output. Then PEST changes the parameter values, reruns the model until the weighted sum of squared errors, the objective function, is minimized. The parameter set that gives the minimum error is the optimum result.

The PEST control file also includes the command that must be executed in order to run the model. In this case, the model command line is ‘iSWAT_2005’. The PEST program uses its template files to change the parameter values in the model input files, runs the model, uses its instruction files to extract the model output and compare it to observations, and calculates the objective function. This entire process is repeated as necessary to explore the parameter space and minimize the objective function within user-specified tolerance.

4.4 DISCHARGE DATA FOR COMPARISON

Comparing the model output with the real data is the essence part of watershed model calibration. Judgment regarding the performance of the model is largely based on whether the model can accurately simulate real data. In this calibration study, real discharge data are of great importance, because PEST needs the comparison results to auto-adjust the model parameter values.

In this work, iSWAT is used to simulate discharge from Nov. 11, 1994, to Oct. 31, 2006. Data from 15 USGS gage stations are selected. Each of these stations has a sub-basin and river reach number. For convenience, each station is given a 3-letter abbreviation (Table 4.5). All of these data are obtained from USGS website. (USGS, 2011)

Table 4.5 The 3-letter Abbreviation for 15 Gaging Stations

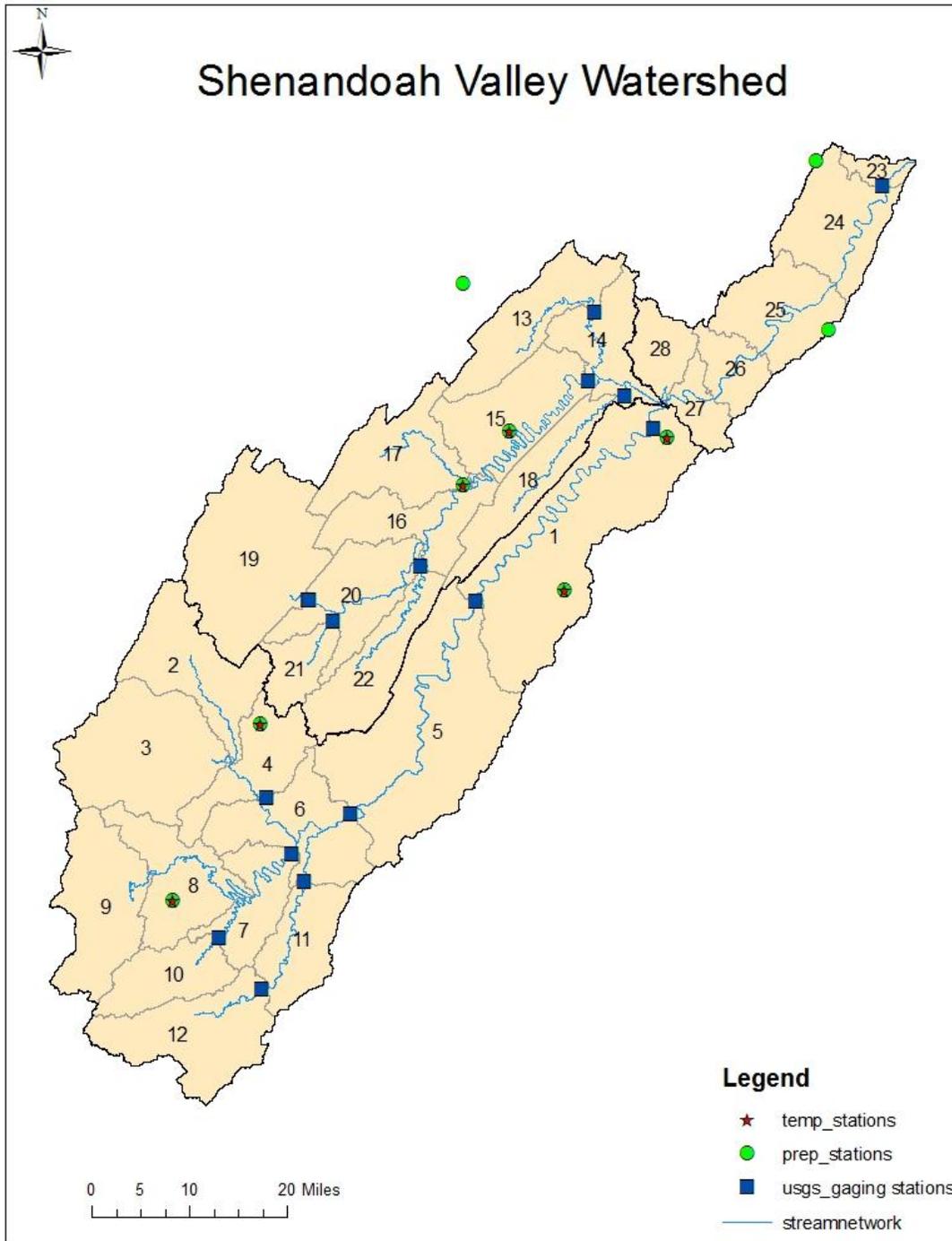
Subbasin	Model Reach	Name of USGS station	3letter ABR.	Duration
0501	1	USGS 01631000 S F Shenandoah River at Front Royal, VA	ssf	1996-2006
0504	4	USGS 01622000 North River near Burketown, VA	nrb	1996-2006
0505	5	USGS 01629500 S F Shenandoah River near Luray, VA	ssy	1996-2006
0506	6	USGS 01628500 S F Shenandoah River near Lynnwood, VA	ssl	1996-2006
0507	7	USGS 01625000 Middle River near Grottoes, VA	mrg	1996-2006
0510	10	USGS 01624800 Christians Creek near Fishersville, VA	ccf	1996-1997
0511	11	USGS 01627500 South River at Harrison, VA	srh	1996-2006
0512	12	USGS 01626000 South River near Waynesboro, VA	srw	1996-2006
0601	13	USGS 01634500 Cedar Creek near Winchester, VA	ccw	1996-2006
0603	15	USGS 01634000 N F Shenandoah River near Strasburg, VA	nss	1996-2006
0606	18	USGS 01635500 Passage Creek near Buckton, VA	pcb	1996-2006
0607	19	USGS 01632000 N F Shenandoah River at Cootes Store, VA	nsc	1996-2006
0609	21	USGS 01632082 Linville Creek at Broadway, VA	lcb	1996-2006
0610	22	USGS 01632900 Smith Creek near New Market, VA	scn	1996-2006
0702	24	USGS 01636500 Shenandoah River at Millville, WV	shm	1996-2006

It should be noted here that PEST is instructed to compare model output with observations only from Jan. 1, 1996, to Oct. 31, 2006. The reason is the model

warm up period. SWAT model needs to run a certain period of time to adjust initial conditions that are likely not consistent with the parameter set and forcings. After that, model states, forcing, and parameters are generally consistent. Therefore, a two-year warming up period is applied for this iSWAT-PEST model. PEST would modify the parameters so as to make the model outputs as close as possible to observations for Water Years 1997 through 2006.

4.5 MODEL SUMMARY

The model setup is summarized graphically in Figure 4.7. This map shows the 28 subbasins, the streams, the 15 USGS gaging stations, the six temperature stations, and the nine precipitation stations.



Produced by: Yan Wang Source: ICPRB Team

Figure 4.7 Summary Map of the Shenandoah Watershed Model

CHAPTER FIVE

GENERAL METHODS FOR MODEL MODIFICATION AND ANALYSIS

This chapter describes the procedure used to calibrate the ICPRB SWAT (iSWAT) Shenandoah Model using PEST. In the whole study process, 16 different calibration attempts were performed. In this chapter, general modification methods are described. Also included are model output analysis methods.

Section 1 describes the meaning of model performance, as applied to all attempts. The remaining sections discuss the approaches to the calibration objective functions, and the selection of adjustable parameters for the different attempts.

The very first calibration is a trial run of the iSWAT Shenandoah Model, excluding the PEST calibration. After the first calibration, each step of the study was designed in response to results from the previous steps.

This chapter outlines the steps. Results are provided and discussed in Chapter 6.

5.1 MEASURES OF MODEL PERFORMANCE

To find the parameter set that results in the best model, it is first necessary to define “best.” This section describes the qualitative and quantitative measures used to judge the model versions that result from different parameter sets and parameter values.

5.1.1 Parameter rationality

The parameter values selected in calibration must be physically reasonable. Adjustable parameters represent properties of the watershed or response unit that cannot be measured. Still, their sign and magnitude must be consistent with the processes believed to be operating the system.

In the ICPRB iSWAT Shenandoah Model, parameters should also be different for the different soil, geology, and vegetation types. For example, the “evaporation efficiency” parameters are expected to be different for crops and forest. The baseflow parameters are expected to be different for limestone regions and sandstone regions.

The evaluation of parameter rationality was carried out using SENSAN package (More detailed descriptions of SEASAN are stated in section 5.5.3). The results and the procedures are described in section 6.6.

5.1.2 Goodness of fit of modeled discharge

Summary statistics are usually applied as a measure of how well the model hydrograph fits, or agrees with, the observed hydrograph. The correlation coefficient R and the coefficient of determination R^2 are important indicators of how well future outcomes are likely to be predicted by a mathematical model.

The correlation coefficient R is an index of the degree of linear association between two random variables. The magnitude of R indicates whether the model provides accurate prediction of the criterion variable. R measures the degree to

which the measured and predicted values agree and is used as a measure of the accuracy of future predictions.

The coefficient of determination R^2 is also a meaningful indicator of the accuracy of predictions. R^2 is the ratio of EV (Explained Variance) to TV (Total Variance). R^2 is a statistic that will give some information about the goodness of fit of a model. In regression, the R^2 is a statistical measure of how well the regression line approximates the real data points. An R^2 of 1.0 indicates that the regression line perfectly fits the data.

Generally, most hydrologic models are not simply linear models. To provide reasonable values and to better use these indicators, R and R^2 can be calculated as

$$R^2 = \frac{EV}{TV} = \frac{\sum_{i=1}^n (\hat{y}_i - \bar{Y})^2}{\sum_{i=1}^n (y_i - \bar{Y})^2} \quad Eq. 5.1$$

$$R = \sqrt{R^2} \quad Eq. 5.2$$

where \hat{y}_i is the i 'th predicted value,

y_i is the i 'th observed value,

\bar{Y} is the mean value for all the observations.

In the iSWAT Shenandoah model, observations from 15 gaging stations are the real data, and the model output surface runoff is the predicted data. The observation data are entered in the PEST control file, as described in section 2.4.3. R^2 can be calculated and used as a index for goodness of fit (Ayyub and McCuen, 1997).

PEST uses a weighted correlation coefficient R_w to evaluate the goodness of fit of the model. The weighted correlation coefficient is independent of the number of observations involved in the parameter estimation process, and is independent of the absolute levels of uncertainty associated with those observations (Doherty, 2004). The R_w value is automatically calculated by PEST.

R_w is defined by Cooley (1990) as:

$$R_w = \frac{\sum_{i=1}^n (w_i y_i - m)(w_i \hat{y}_i - m_o)}{[\sum_{i=1}^n (w_i y_i - m)(w_i y_i - m) \sum_{i=1}^n (w_i \hat{y}_i - m_o)(w_i \hat{y}_i - m_o)]^{1/2}} \quad Eq. 5.3$$

where \hat{y}_i is the i 'th predicted value,

y_i is the i 'th observed value,

w_i is the user-assigned weight associated with the i 'th observation,

m is the mean value of weighted observations,

m_o is the mean of weighted model-generated counterparts to observations.

In this study, both the weighted and non-weighted correlation coefficients are calculated and used as a measurement of goodness of fit. The weighted correlation coefficients are calculated from Jan. 1st, 1996, to Oct. 31st, 2006, incorporating all 15 discharge observation groups (USGS gauge daily discharge records) and their corresponding model predictions. The non-weighted correlation coefficients are calculated from Nov. 1st, 1996, to Oct. 31st, 2006, incorporating all 15 observation groups and their corresponding model predictions. The weighted R and the non-weighted R are two different measurements of goodness of fit. The two are identical when all the weights are set to 1.0, but otherwise not comparable. Therefore, comparisons are not

performed between the weighted and the non-weighted R in each model version. However, the two types of R are compared among versions, respectively.

5.1.3 Nash-Sutcliffe coefficients

The Nash–Sutcliffe model efficiency coefficient (NSE) is used to assess the predictive power of hydrological models (Nash, 1970). It is defined as:

$$E = 1 - \frac{\sum_{t=1}^T (Q_0^t - Q_m^t)^2}{\sum_{t=1}^T (Q_0^t - \overline{Q_0})^2} \quad \text{Eq. 5.4}$$

where Q_0 is observed discharge,

Q_m is modeled discharge.

Q_0^t is observed discharge at time t .

Nash–Sutcliffe efficiencies can range from $-\infty$ to 1. An efficiency of 1 ($E = 1$) corresponds to a perfect match of modeled discharge to the observed data. An efficiency of 0 ($E = 0$) indicates that the model predictions are as accurate as the mean of the observed data, whereas an efficiency less than zero ($E < 0$) occurs when the observed mean is a better predictor than the model or, in other words, when the residual variance (described by the numerator in the expression above), is larger than the data variance (described by the denominator). Essentially, the closer the model efficiency is to 1, the more accurate the model is.

It should be noted that Nash–Sutcliffe efficiencies can also be used to quantitatively describe the accuracy of model outputs other than discharge. This method can be used to describe the predictive accuracy of other models as long as there is observed data to compare the model results to. For example, Nash–Sutcliffe efficiencies have been reported in scientific literature for model

simulations of discharge and water quality constituents such as sediment, nitrogen, and phosphorus loadings.

NSE is similar to R^2 . However, NSE uses the percentage of unexplained variance to total variance as an indicator of goodness of coefficient, and NSE is widely used in hydrologic model verification (Nash, 1970). It should be noted that NSE, as a single-value index, can be sensitive to a number of factors, such as sample size, outliers, magnitude bias, and time off-set bias (McCuen et al., 2006). For a non-linear model, negative NSE can result even when the model is unbiased (McCuen et al, 2006). Therefore, a low value of NSE may not necessarily mean a poor model, and it cannot be used as a single index for model evaluation. The NSE can still be a judgment of goodness of fit as long as it can be properly interpreted.

In this iSWAT-PEST model evaluation, the average observed discharge \overline{Q}_0 is assigned a slightly different meaning. \overline{Q}_0 is not the overall average discharge throughout the observation years. Rather, it is the average annual discharge hydrograph (Maidment, 1993). The reason for using these average values is to account for seasonal trend in river flows. The rationale is that an analyst would not typically use a single average annual value as a first estimator for stream discharge, but would used the average annual hydrograph instead.

Several steps were taken to obtain the average values.

- 1) Average the discharges on the same date in each year.

For example, there are 10 years of record of discharge in reach 24. The 10 values reported on on October 30th are averaged. Applying the same procedure for the other 364 days gives the average daily discharge for each day of the year can be obtained; this time series is defined as the average annual hydrograph.

Example calculations are shown in Table 5.1.

Table 5.1 Sample Calculation of Average Daily Discharge (cfs)

MM	DD	1996	1997	1998	1999	2000	2001	2002	2003	2004	2005	2006	Mean Daily
1	1	N/A	4080	1850	590	1870	980	400	2960	4700	2930	3680	2404
1	2	N/A	3930	1800	600	1840	960	385	11500	4430	2790	3540	3178
1	3	N/A	3820	1810	760	1780	945	370	15700	4210	2690	3990	3608
1	4	N/A	3720	2010	712	1720	930	360	12000	4020	2490	4270	3223
1	5	N/A	3520	2540	924	1700	915	350	9890	3850	2540	4040	3027
1	6	N/A	3430	3050	1200	1580	900	340	7980	3740	2470	3740	2843
1	7	N/A	3290	3490	1280	1540	890	400	6690	3560	2500	3440	2708

Observations from Nov. 1st, 1996, to Oct, 31st, 2006. Therefore, there are missing data in years 1996 and 2006; however, each day of the year has ten years of measurements (with the exception of Feb 29).

2) Smooth the noisy daily averaged values.

In order to get a smooth yearly trend, a moving average filter is employed. A moving window of 31 days is used. The results are shown in Figure 5.1. The blue line represents the averaged values calculated from previous step. The red one indicates the smoothed values.

This example is a clear seasonal trend in discharge. Late winter/ early spring (from February to April) has high discharge while summer (July -August) has low flow. A secondary peak in late summer/early (from September to October) fall reflects the tropical storm/hurricane season in this region.

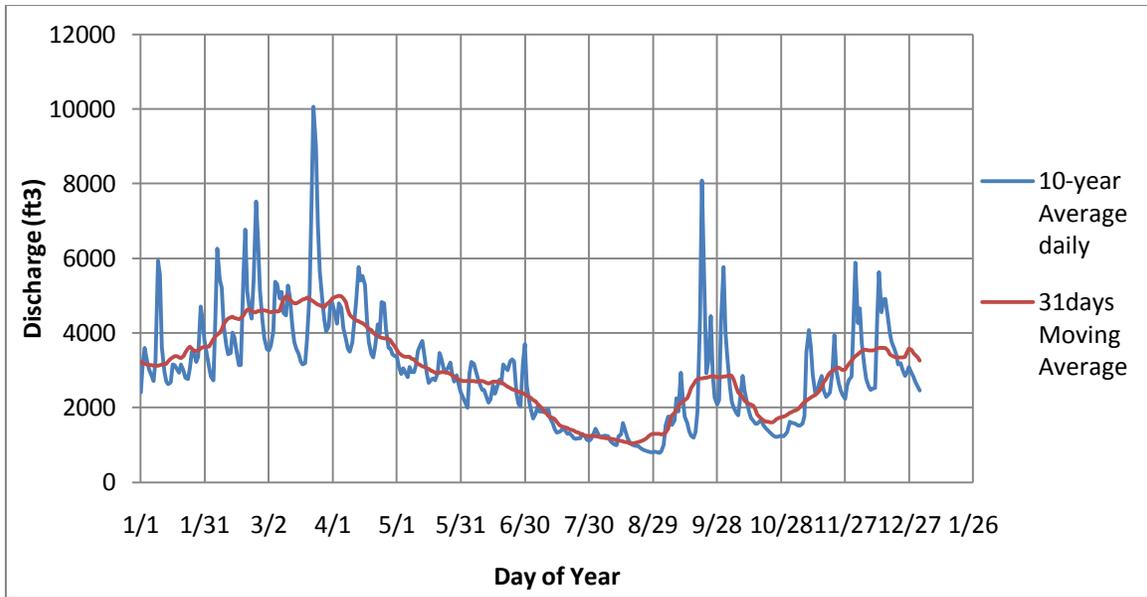


Figure 5.1 Moving Average Filter for Daily Average Discharge (31 steps)

3) Then the NSE equation can be modified into

$$E_m = 1 - \frac{\sum_{t=1}^T (Q_0^t - Q_m^t)^2}{\sum_{t=1}^T (Q_0^t - \bar{Q}_i)^2} \quad \text{Eq. 5.5}$$

where \bar{Q}_i is the ordinate of the smoothed average annual hydrograph corresponding to time t , $i = 1, 2, \dots, 365$ (366 for Leap Year). The modified NSE (Eq. 5.5) is applied to each stream gauge individually.

The application of E_m instead of E in this study makes it a more demanding test for the modeled output. Since \bar{Q}_i is a better estimator of daily discharge than \bar{Q}_0 , the value of the denominator in Eq. 5.5 $\sum_{t=1}^T (Q_0^t - \bar{Q}_i)^2$ is smaller than that of the denominator in Eq. 5-4 $\sum_{t=1}^T (Q_0^t - \bar{Q}_0)^2$, with the result that the subtracted term in Eq. 5-5 is larger than that in Eq. 5-4. Therefore, given the same data set, E_m is smaller than E . If E_m indicates a good model, then it gives more confidence in the accuracy of the model.

5.1.4 Other criteria

Summary statistics are not the only evaluation criteria for hydrologic models. Other important factors for judging the performance of such models include specific characteristics of the patterns of streamflow, as shown in the observed hydrograph. The model hydrograph should reproduce these patterns as closely as possible.

1) Peak discharge

High flows are the result of heavy precipitation or snowmelt. An accurate model captures both the magnitude and the timing of peak flow.

2) Recession

The recession curve is the specific part of the flood hydrograph after the crest (and the rainfall event) where streamflow diminishes (Connected Water, 2006). The slope of the recession curve flattens over time from its initial steepness as the quick flow component passes and baseflow becomes dominant. A recession period lasts until stream flow begins to increase again due to subsequent rainfall. Hence, recession curves are the parts of the hydrograph that are dominated by the release of water from natural storages, typically assumed to be groundwater discharge. Recession segments can be selected from the hydrograph and can be individually or collectively analyzed to gain an understanding of these discharge processes that make up baseflow (Connected Water, 2006).

Each recession segment is often considered as a classic exponential decay function as applied in other fields such as heat flow, diffusion or radioactivity, and expressed as:

$$Q_t = Q_o e^{-\frac{t}{T_c}} \quad \text{Eq. 5.6}$$

where Q_t is the stream flow at time t

Q_o is the initial stream flow at the beginning of recession (peak discharge)

T_c is the resident time of the groundwater system.

As discussed in section 3.3, the exponential recession equation 5.6 implies linear reservoir behavior, which may or may not be appropriate for the Shenandoah Watershed.

Hydrographs created using the modeled discharge output should have similar recession slopes to observed hydrograph. The slope (and slope change) in recession is an indicator of watershed response. Although the model does not simulate the subsurface flow in detail, it should capture the general behavior.

3) Annual total discharge

Model calculated annual total runoff should not have much difference from the actual observations. A difference with a value of 2 inches is usually acceptable (McCuen, 2010).

4) Annual water balance

The water balance in this model can be approximately expressed as

$$\text{Change in Storage} = \text{Precipitation} - \text{Runoff} - \text{Evapotranspiration}$$

Although total water storage in a watershed changes throughout the year, it is generally reasonable to assume that the change over a water year is small (where the water year begins at the time of minimum storage, by definition). Generally, a calculated change in storage with a value of 2 inches is considered a good prediction (i.e., good model performance) (McCuen, 2010)

5.2 WEIGHTED OBJECTIVE FUNCTION

In PEST, the objective function is weighted sum of squared residuals. The user applies knowledge of the watershed and observational data to define the weights in the PEST control file. Users are free to set the weights according to their own judgment, and may wish to experiment with different weighting schemes. For the same parameter set, different sets of weights will result in different values of the weighted R_w (Eq. 5.3), and allowing the optimization to minimize R_w with a different set of weights will generally result in a different parameter set. As discussed in section 5.1.2, the two values of R_w cannot be directly compared; whether one parameter set is superior to the other must be judged using the other criteria described in Section 5.1.

In some models, observed data may be given in different units (for example, a model might predict discharge and water temperature or concentration); the weights allow the user to scale the squared residuals to the same order of magnitude. In the Shenandoah SWAT model, all observations are stream flow in cfs.

It is possible to assign a different weight to each day in the observation time series. For this study, however, different weights were assigned to the 15 gauging stations. For a given gauge, every day in the observation time series was assigned the same weight.

In the 28 subbasins, 28 reaches are defined. Although the subbasin areas are approximately the same, the reach lengths and discharge rates are different. Some reaches are main channels in the subbasin, whereas in the whole watershed, they are only tributaries. Water from all tributaries flows to the main reach, which results in a great difference (even several orders of magnitude) between flow rate in the main channel and in the tributary channels.

As discussed above (Chapter 2.2.3), equally weighting all of these observations allows the quantity represented by the larger numbers to take undue precedence in the estimation process (Doherty, 2004). In this case, it is possible that PEST would ignore the small rivers, resulting in inaccurate calibration. Therefore, observation weightings are of great importance for this model calibration process.

Different weighting methods are explored in this work. It should be noted that the model is ultimately judged by the criteria enumerated in section 5.1. The judging criteria (NSE, non-weighted R^2 , water balance, etc.) are not used as objective functions in the calibration.

1) Equal weights

First, the 15 observation groups from the 15 USGS gaging stations are assigned equal weights of 1.0. Equal-weight is the most basic weighting method used in modeling. This method gives all residuals the same importance in the sum of squared residuals, without regarding the differences in magnitudes (and /or units) of the observations.

2) Weights assigned by residuals

The PEST output record file for the equal weights run summarizes the total sum of squared residuals and contributions from each observation group.

According to the magnitude rules, a greater contribution to total sum of squared residuals means that parameter adjustment did not favor correct prediction at that gauge. The next method was devised to force that gauge's observation group to have greater precedence in the objective function.

Therefore, the new weights were assigned by:

$$\text{new weight } i = \frac{\text{contribution of the observation group } i}{\text{total sum of squared weighted residuals}} \cdot k1 \quad \text{Eq. 5.7}$$

where i represents the i 'th observation group,

$k1$ is a constant factor selected to scale the weights for convenient text entry in the PEST control file (relative weights are unchanged).

3) Weights assigned by daily average discharge rate

Due to their different sizes, stream orders, and environmental conditions, flow rate in different reaches is different. Although there is seasonal variation

of baseflow and different response to precipitation, average discharge can be a good representation of the general flow quantity condition in each river. The weights assigned to observations should reflect the relative magnitudes of the numbers used to express the quantities (Doherty, 2004). Therefore, daily average discharge rate for the period from Nov. 11, 1994, to Oct. 31, 2006, are calculated for each observation group (gage):

$$Ave_Qi = \frac{\sum \text{daily daily discharge from gaging station } i}{\text{total number of days}} \quad Eq. 5.8$$

where i represents the i^{th} observation group.

The new weights for each observation group are inversely proportional to the daily average discharge for each reach.

$$\text{new weight } i = \frac{1}{Ave_Qi} \cdot k2 \quad Eq. 5.9$$

where i represents the i^{th} observation group,

$k2$ is a constant factor selected to scale the weights for convenient text entry in the PEST control file (relative weights are unchanged).

This approach increases the influence of the smaller streams.

4) Weights assigned by standard deviation of discharge rate

Flow in different reaches exhibits different standard deviation, which reflects the degree each discharge rate differs from its average. To reflect the different variances, another weighting method is employed.

The standard deviation of daily discharge can be calculated as

$$Sd_{Qi} = \sqrt{\frac{\sum(\text{observations} - \text{mean daily discharge})^2}{\text{total number of days} - 1}} \quad \text{Eq. 5.10}$$

where i represents the i' th observation group.

The new weights for each observation group are inversely proportional to the standard deviation for each reach.

$$\text{new weight } i = \frac{1}{Sd_{Qi}} \cdot k3 \quad \text{Eq. 5.11}$$

where i represents the i' th observation group,

$k3$ is a constant factor selected to scale the weights for convenient text entry in the PEST control file (relative weights are unchanged).

This approach increases the influence of the less-variable streams.

5) Weights assigned by an ordinal-scale

In this weighting method, a flow-direction chart is created to identify which reaches are the tributaries and which are the main streams. The flow network is determined from the watershed map. The flow-network chart is shown in Figure 5.2. Each box represents a reach. The numbers in the box are the reach numbers identified by SWAT (subbasin numbers).

Here, the reaches are classified into 11 ordinal values based on the stream network. The most upstream ones are the 11th level and the most downstream one is the 1st level. The level of each upstream reach is determined by the number of flow links through the network to the outlet. For example, reach 7 is defined as level 9 because the flow follows links 7-6-5-1-27-26-25-24-23 (nine

links); reach 28 is defined as level 6 because its flow follows links 28-27-26-25-24-23 (six links). The new weights are assigned to each reach by

$$\text{new weight } i = (\text{level of reach } i) \cdot k4 \quad \text{Eq. 5.12}$$

where i represents the i 'th observation group,

$k4$ is a constant factor selected to scale the weights for convenient text entry in the PEST control file (relative weights are unchanged).

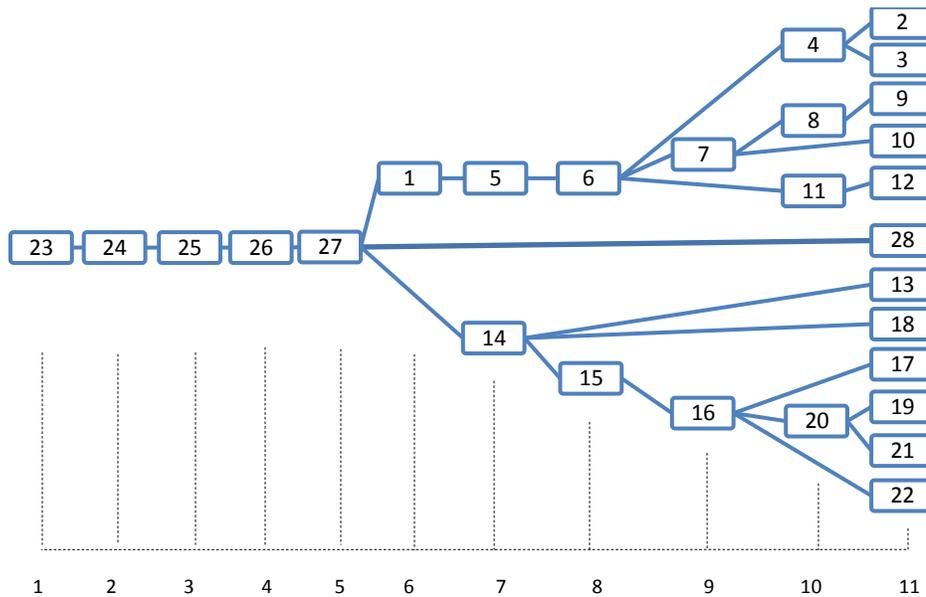


Figure 5.2 Flow-network Chart for Ordinal Scale

Table 5.2 shows the mean and standard deviation of discharge of each reach. Table 5.3 lists the specific weights assigned to each observation group using the different weighting method.

5.3 INCREASING THE NUMBER OF ADJUSTABLE PARAMETERS

In the first version of calibration (V2 in this study; V1 is just a run of iSWAT without coupling with PEST), only the roughness coefficients for main channels and tributary channels, and the overall basin-scale parameter “SURLAG” were

modified. Five roughness coefficient values for tributaries and five for the main channels were adjustable, as described in section 4.3.

In the second calibration attempt (V3), three parameters of the groundwater module (Groundwater delay, Alpha parameter, and Beta parameter) were adjustable. These parameters were assigned to the HRUs by geology (section 4.1), so that instead of separately estimating them for each HRU (489X3 parameters), 21 groundwater parameters were adjusted. It was expected that including these parameters would improve baseflow and hydrograph recessions.

Table 5.2 Mean and Standard Deviation of Reach Discharge(cfs)

River Name	Reach	Mean Discharge	Standard Deviation	Coefficient of Variation
South Fork Shenandoah River at Front Royal	1	45.76	64.04	1.40
North River near Burketown	4	11.32	15.26	1.35
South Fork Shenandoah River near Luray	5	40.87	62.10	1.52
South Fork Shenandoah River near Lynnwood	6	29.88	44.08	1.48
Middle River near Grottoes	7	9.12	13.85	1.52
Christians Creek near Fishersville	10	2.20	5.05	2.30
South River at Herriston	11	7.29	12.63	1.73
South River near Waynesboro	12	4.43	7.78	1.76
Cedar Creek near Winchester	13	2.91	5.35	1.84
North Fork Shenandoah River near Strasburg	15	18.16	25.68	1.41
Passage Creek near Buckton	18	2.26	4.58	2.03
North Fork Shenandoah River at Cootes Store	19	5.60	12.24	2.19
Linville Creek at Broadway	21	1.09	2.27	2.08
Smith Creek near New Market	22	2.17	3.91	1.80
Shenandoah River at Millville	24	83.79	108.64	1.30

Finally, parameters controlling evapotranspiration and interception were freed for adjustment in Version 3m. Evapotranspiration related parameters include Soil evaporation compensation factor, Slope length for lateral subsurface flow, and Plant uptake compensation factor. Interception related parameters are maximum canopy storage. Soil evaporation compensation factor and Slope length were assigned to the HRUs by geology (section 4.1); Plant uptake compensation factor and maximum canopy storage are assigned by land use (two classes are defined: crop and forest). Therefore, there were total of 22 evapotranspiration parameters and 2 interception parameters being adjusted in each version starting from Version 3m.

Table 5.3 Weights Assigned to Each Observation Group

Observation Group	Reach Number	WM1	WM2	WM3	WM4	WM5
		V3	V4,V5	V6,V7	V8	V9-V16
South Fork Shenandoah River at Front Royal	1	1.000	0.003	0.002	0.035	0.583
North River near Burketown	4	1.000	0.021	0.014	0.149	0.917
South Fork Shenandoah River near Luray	5	1.000	0.004	0.003	0.037	0.667
South Fork Shenandoah River near Lynnwood	6	1.000	0.006	0.004	0.052	0.750
Middle River near Grottoes	7	1.000	0.050	0.033	0.164	0.833
Christians Creek near Fishersville	10	1.000	1.054	0.699	0.450	1.000
South River at Herriston	11	1.000	0.060	0.040	0.180	0.917
South River near Waynesboro	12	1.000	0.184	0.122	0.292	1.000
Cedar Creek near Winchester	13	1.000	0.251	0.166	0.424	1.000
North Fork Shenandoah River near Strasburg	15	1.000	0.009	0.006	0.088	0.750
Passage Creek near Buckton	18	1.000	0.269	0.178	0.496	1.000
North Fork Shenandoah River at Cootes Store	19	1.000	0.040	0.027	0.185	1.000
Linville Creek at Broadway	21	1.000	1.603	1.062	1.000	1.000
Smith Creek near New Market	22	1.000	0.572	0.379	0.582	1.000
Shenandoah River at Millville	24	1.000	0.001	0.001	0.021	0.167

Table 5.4 Number of Adjustable Parameters in Each Version

Para.	Meaning	No. of adjustable parameters					
		V2	V3-V4	V3m&V5&V6	V7-V9	V10	V11-V16
Surlag	Surface runoff coefficient	1	1	1	1	1	1
n1	Manning's n value for tributary channels	5	5	5	6	---	6
n2	Manning's n value for main channels	5	5	5	5	---	---
gd	Groundwater delay		7	7	7	7	7
a	Baseflow Alpha parameter		7	7	7	7	7
b	Baseflow Beta parameter		7	7	7	7	7
s	Soil evaporation compensation factor			10	10	10	10
e	Slope length for lateral subsurface flow			10	10	10	10
epco	Plant uptake compensation factor			2	2	2	2
can	Maximum canopy storage			2	2	2	2

--- means the parameter is included in the PEST control file, but held fixed

Blank means the parameter is not included in the PEST control file.

5.4 SELECTION OF ADJUSTABLE PARAMETERS

Over parameterization is a major problem in hydrologic modeling processes (Doherty, 2004). On the one hand, including many free parameters can improve the agreement with measurement; in the other hand, adjustment of many parameters can be time consuming. In addition, high inter-correlation of parameters reduces the model prediction value. Therefore, reducing the number of parameters (dimension of parameter space) in a proper manner may lead to better model calibration results.

As discussed in section 5.3, the iSWAT Shenandoah model has hundreds of parameters. Several dozen of these are subbasin or HRU properties that cannot be measured or determined from geographic information. These parameters

include physical properties such as channel roughness coefficients (Manning's n values), as well as coefficients of conceptual process representations, such as α and β parameters in the groundwater module. The complete list of adjustable parameters is given in Table 5.1.

In this iSWAT model, a number of 0.07 is the initial guess for all main channel roughness coefficients, and they are constrained to from 0.025 to 0.16 (range provided by SWAT manual). Then PEST was employed to estimate the best main channel roughness (n_2) for the various geology types. The n_2 values vary in each trial but the resulting n values in some cases their rationality was suspect. An example of a set of irrational n_2 values are shown in Figure 5.3

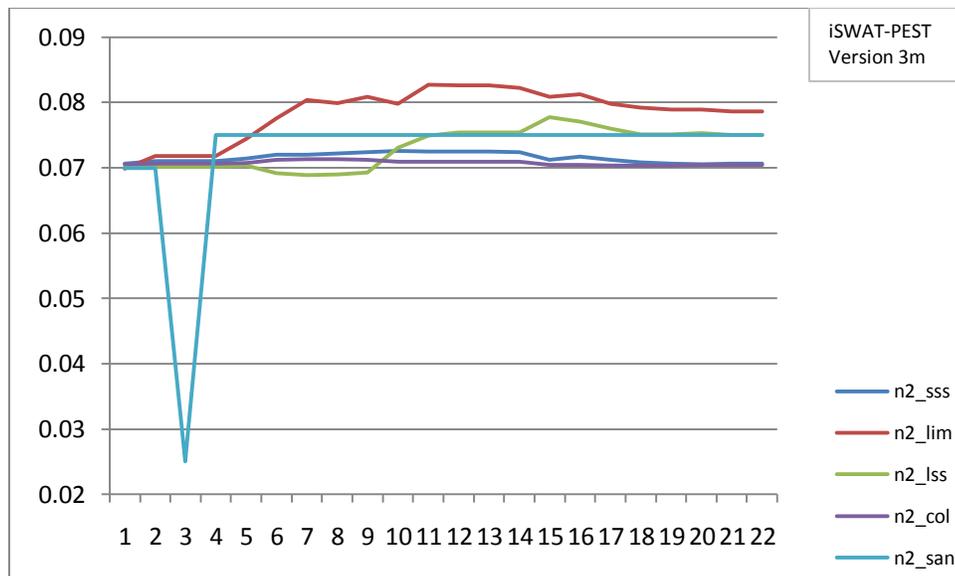


Figure 5.3 Parameter value change through iteration process

This figure shows that all the roughness coefficients are approximately the same value of 0.075, which is irrational for a watershed bearing various soil types and vegetations. Therefore, another method was considered to estimate the

roughness coefficients and have them fixed (not changeable) in PEST calibration processes. This method is discussed below.

1) Estimating hydraulic properties

McCandless (2003) proposed a set of regression equations for bankfull discharge and channel characteristics in the Allegheny Plateau and Valley and Ridge Hydrologic Regions. The study area in this research is within the range of where these equations can be applied. Therefore, the regional regression equations are employed to obtain main channel roughness coefficients.

The basic concept is to 1) use the regression equations to get channel characteristics, 2) use Manning's Equation to calculate the roughness coefficient.

$$Q = 34.02DA^{0.94} \quad \text{Eq. 5.13}$$

$$A = 13.17DA^{0.75} \quad \text{Eq. 5.14}$$

$$W = 13.87DA^{0.44} \quad \text{Eq. 5.15}$$

$$Y = 0.95DA^{0.31} \quad \text{Eq. 5.16}$$

where DA --- Drainage area

Q --- Bankfull discharge

A --- Bankfull cross-section area

W --- Bankfull top width

Y --- Bankfull depth

Equations 5.13 through 5.16 are the empirical relationships derived by McCandless (2003). Solving the Manning's equation for the roughness coefficient n , gives the following expression

$$Q = V \cdot A = \frac{1.49}{n} R^{2/3} S^{1/2} = \frac{1.49}{n} \frac{A^{5/3}}{(W + 2Y)^{2/3}} \left(\frac{Re}{L}\right)^{1/2} \quad Eq. 5.17$$

$$n = \frac{1.49}{Q} \frac{A^{5/3}}{(W + 2Y)^{2/3}} \left(\frac{Re}{L}\right)^{1/2} \quad Eq. 5.18$$

where Re --- Elevation relief from channel head to mouth

L --- Reach length

V --- Velocity

The quantities on the right-hand side of Eq. 5.18 can either be obtained from GIS or estimated using the McCandless (2003) empirical equations.

2) Using GIS to get the needed information

For each reach, the drainage area (watershed area), maximum elevation and minimum elevation along the reach and the length of the reach are obtained using GIS.

i. Obtaining the watershed area

Download the elevation and hydrology (stream) information from the USGS Seamless Server (USGS, 2010).

Load the information into ArcGIS. Set proper projected coordinate system.

Fill the elevation raster, calculate flow direction and flow accumulation to get the stream network.

Locate on map the designed outlets in iSWAT model.

Delineate the watershed for each outlet.

Due to the characteristic of watershed delineation, some basic math (subtraction) is needed to get the drainage area for each sub-watershed.

ii. Obtaining the reach relief

Use Identify Tool to identify the elevation of the most upstream and the most downstream point of the reach. The relief should be

$$Re = E_{max} - E_{min} \quad Eq. 5.19$$

where E_{max} --- Maximum elevation of the stream (meters);

E_{min} --- Minimum elevation of the stream (meters);

iii. Obtaining the reach length

The streams provided by the USGS Seamless Server are just the main streams. Based on the outlets, GIS operations Merge and Split are needed to divide the streams. By recalculate geometry--- length (in meters) of the resulting stream segments, the reach length can be obtained.

3) Post processing

Having obtained all the information needed, data processing can be continued in a spread sheet using the Regression Equation and the Manning's Equation.

The roughness coefficients are then calculated. The new roughness coefficients for main channels resulting from this analysis are listed in Chapter 6.

4) Discussion

In the analysis and calculation process, the subbasin areas, the stream reach length, and the stream reach reliefs differs from those applied in the iSWAT model (shown in the maps for each HUC as provided by the ICPRB team) are different from those provided by the GIS analysis. Taking HUC 06 (NF_Shen) as an example. In GIS, ten designated outlets (red pts) were located on/near the streams, shown in Figure 5.4. Compared to the map in Figure 5.5, the lengths of reach 1, 5, 6, 7, 9, 10 (the most upstream reaches) are much greater.

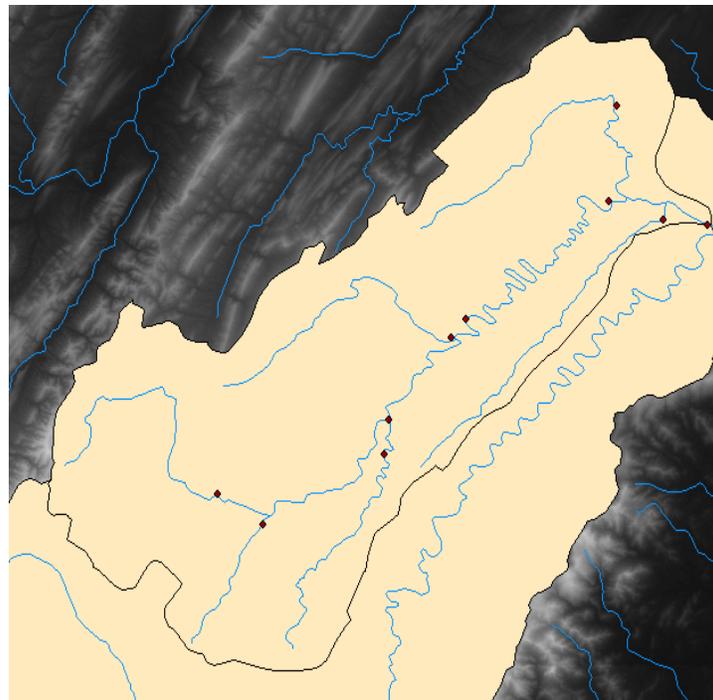


Figure 5.4 USGS Seamless Server Main Channels

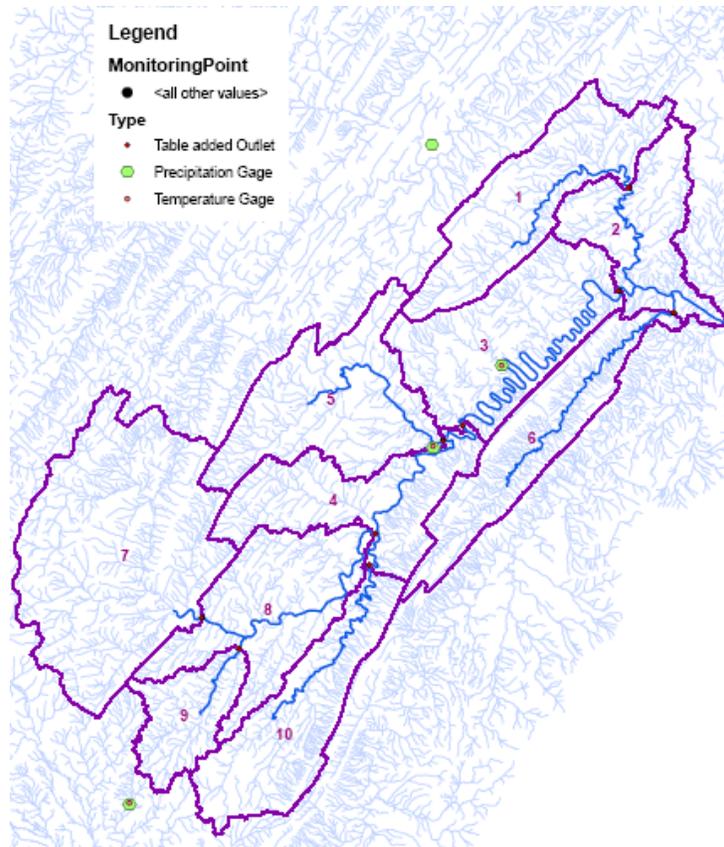


Figure 5.5 Reaches provided by ICPRB team (ArcSWAT analysis)

Table 5.5 tabulates the different reach lengths, slopes and subwatershed areas. The highlighted rows are the most different ones. Some reaches are significantly longer in the more recent GIS analysis but others are shorter.

One possible reason for the differences may be that different threshold values are used to define the main channel. This difference in threshold values would result in difference in reach length and reach relief, resulting in large differences in some upstream reaches (in the mountainous regions).

If the new n values are to be used in further runs, the reach lengths and slopes should also be changed in the .rte files and .ptf files, as well as drainage areas in .sub files.

5. 5 EXPLORATION MADE WITHIN PEST

In addition to using PEST in calibration mode to estimate the parameters of the iSWAT Shenandoah model, some other modeling tools available in the PEST package were also explored: Predictive Analysis and Regularization.

5.5.1 Using Predictive Analysis Mode in PEST auto-calibration process.

As discussed above, the existence of local optima is a major problem in hydrologic modeling. It is quite normal that several sets of parameters could result in the minimum value (or very close to the minimum) to the objective function but give different predictions at the same time. Therefore, the selection of the parameter set does not only depend on objective function, but also the prediction values. In some cases, modelers may need the parameter set that could result in the minimum prediction; or the set that could result in the maximum predictions. PEST can address this problem.

In predictive analysis mode, PEST aims to maximize or minimize a specified prediction while maintaining the model in a calibrated state (ensuring that the objective function rises no higher than a specified level). In this mode, PEST is allowed to have higher objective function value than that in estimation mode. An observation must be specified to allow PEST to predict the max/min value of this observation within the acceptable parameter sets.

In the very first several iSWAT runs, reach 13 showed generally high degree of underestimation for runoff. Therefore, the most deviate observation in reach 13 is set as a single observation group “predict” as required by the PEST Prediction

Mode. PEST was asked to maximize the calculated value of this group while keeping a relatively high level of significance in the objective function.

Table 5.5 Lengths and Slope Differences

Subbasin	SWAT_INPUT			GIS		
	Length(Km)	Slope(m/m)	Area (m2)	Length(Km)	Slope(m/m)	Area(m2)
501	92.81	0.001	732.536	77.5	0.003	776.501
502	24.335	0.008	241.183	9.025	0.011	311.724
503	6.357	0.002	445.261	21.772	0.005	452.996
504	13.05	0.001	190.514	10.884	0.004	211.183
505	85.35	0.001	745.032	64.119	0.001	760.087
506	25.48	0.001	310.563	28.739	0.001	309.951
507	54.186	0.001	177.521	35.423	0.001	179.289
508	50.61	0.001	267.309	39.609	0.002	268.344
509	13.279	0.003	327.272	29.577	0.005	331.669
510	10.106	0.002	186.614	26.462	0.008	188.084
511	33.548	0.001	188.631	25.453	0.002	203.531
512	25.593	0.001	332.050	35.955	0.005	346.154
601	28.308	0.002	253.589	32.216	0.011	264.322
602	17.815	0.005	165.981	27.186	0.003	194.009
603	78.351	0.001	293.401	54.919	0.001	305.979
604	28.202	0.001	283.887	29.463	0.001	233.371
605	30.794	0.003	283.887	39.453	0.01	291.700
606	40.119	0.003	209.601	44.99	0.011	224.060
607	5.541	0.002	514.929	37.81	0.012	544.645
608	38.149	0.002	258.885	30.516	0.005	264.189
609	12.755	0.003	111.014	18.012	0.006	115.606
610	41.386	0.001	223.332	34.603	0.005	242.786
701	7.971	0.002	55.651	8.767	0.001	44.520
702	27.822	0.001	247.017	27.423	0.001	277.703
703	29.887	0	244.161	26.956	0.001	258.537
704	16.838	0.001	109.897	13.345	0	116.545
705	13.925	0.001	86.260	11.9	0	92.582
706	3.897	0.001	135.182	13.352	0.002	121.979

The problem with this analysis mode is that only one observation can be assigned the predict group. In this study, there are over 50,000 observations.

Maximizing/ minimizing the chosen observation may not assert too much effect

on other predictions. Moreover, even if it does help, problem comes when deciding which one be chosen the predict observation group.

5.5.2 Using Regularization Mode in PEST auto-calibration process.

PEST sometimes encounters difficulties in minimizing the calibration objective function where too many parameters must be simultaneously estimated. In many cases, the modeler would like to include as many parameters as possible in fear that they may lose important model details. However the use of too many parameters typically leads to numerical instability and non-uniqueness of parameter estimates.

A related problem in working with highly-parameterized systems is that depending only on objective function value would result in extreme and even unrealistic predictions. The overall statistics regarding goodness of fit is good. However, system noise may occur as a result. Therefore, some constraints should be imposed on parameter values, or on relationships between parameter values. Moreover, modelers may want to make some parameters as close as possible to preferred values, which are obtained empirically or are based on physical process. Hence an appropriate level of misfit between model outputs and field data can be tolerated as long as the preferred values or the constraints are met.

In regularization mode, PEST aims to maximize adherence to a certain “regularization condition” (by minimizing a regularization objective function) while ensuring that the measurement objective function rises no higher than a specified

level. Reach 13 is always the most problematic one. Therefore, observations in reach 13 are set as the regularization group required by PEST. PEST would try to adhere to all observations in reach 13 while keeping the objective function low.

5.5.3 SENSAN package

SENSAN is a tool package in PEST to carry out sensitivity analysis. Several sets of parameters can be applied to the SENSAN control file at the same time. Then PEST uses each set of parameters to run the iSWAT model one time. The output from each model run would be used as input files for SENSAN to do sensitivity analysis of parameters. The first set of parameters provided in SENSAN control file is set as the base set. All outputs from other sets of parameters are compared to the output from this particular parameter set.

SENSAN requires four types of input files: SENSAN control file, parameter variation file, PEST template file and instruction file. The latter two types of input files are described in section 2.4.3. Parameter variation file include several sets of user specified parameter values. These parameters are identified in the PEST template files. A base parameter set should be provided as the first parameter set (line 2) in the file. This base set is used for comparison (section 5.1).

SENSAN control file supplies SENSAN with the names of all template and instruction files together with the model input/output files to which they pertain. It also provides SENSAN with the model name, field or laboratory measurements to which model outcomes must be matched, and a number of SENSAN variables which control the implementation of the optimization method.

SENSAN generates three output files. The first one (ABSFLE) lists all parameter set values and modeled output for each particular parameter set. The second file (RELFLE) lists the relative differences between the modeled outputs and the observation value provided in control file for each parameter set (equation 5.20). The second file (SENSFLE) provides model outcome sensitivities with respect to parameter variations from their base values (equation 5.21).

$$\frac{O_p - O_b}{O_b} \quad \text{Eq. 5.20}$$

$$\frac{O_p - O_b}{\Delta P} \quad \text{Eq. 5.21}$$

where O_b is the output from base parameter set,

O_p is the output from one parameter set,

ΔP is the difference between perturbed and base parameter values.

In this study, SENSAN is used not only for sensitivity analysis (explained in section 5.1); it is also used for subjective optimization. Because of large amount of SWAT input files, SENSAN is used to re-write all files needed in SWAT and give output files in an easy way. The employment of the package is to carry out subjective optimization.

First, parameters are sorted by parameter types (groundwater parameter or surface runoff parameter) and watershed characteristics (soil type and landuse). Then, they are manually adjusted according to the model performances, such as

peak flow, base flow and runoff recession. A detailed record of the parameter classification and subjective optimization procedure is listed in para_rec.elsx.

Table 5.6 Classification of Parameters

reach	n1 type	n2 type	gw type	a type	b type	evapo type	slope type	plant co	canopy
1	Col	col	col sss lss cry	col sss lss cry	col sss lss cry	3,4,6,16,	3,4,6,16,	c f	c f
4	Col	col	lss	lss	lss	2,3	2,3	c f	c f
5	Col	col	col lss san cry	col lss san cry	col lss san cry	3,4,5,6,	3,4,5,6,	c f	c f
6	Col	col	col lss san	col lss san	col lss san	3,4,5,	3,4,5,	c f	c f
7	Col	col	sss lss	sss lss	sss lss	1,2,3	1,2,3	c f	c f
10	Sss	sss	lss	lss	lss	2,3	2,3	c f	c f
11	Col	col	col lss san cry	col lss san cry	col lss san cry	3,4,5,6,	3,4,5,6,	c f	c f
12	Col	col	col lss cry	col lss cry	col lss cry	3,4,6,	3,4,6,	c f	c f
13	Sss	sss	sss san	sss san	sss san	5,66,	5,66,	f	f
15	Sss	sss	col sss san	col sss san	col sss san	1,2,4,5,66	1,2,4,5,66	c f	c f
18	Sss	sss	sss san	sss san	sss san	1,5,	1,5,	f	f
19	Col	col	col sss san	col sss san	col sss san	1,4,5,	1,4,5,	f	f
21	Lim	lim	lss	lss	lss	2,3	2,3	c f	c f
22	Lim	lim	lss san	lss san	lss san	3,5,	3,5,	c f	c f
24	Col	col	san	san	san	5,66,	5,66,	c f	c f

5.6 CHAPTER SUMMARY

In summary, 16 calibrations were performed. Each calibration attempt was a unique combination of a) a weighting scheme, b) a set of adjustable parameters and c) a PEST optimization mode (estimation, prediction, or regularization).

For each calibration, a PEST control file was created dictating the adjustable parameters, the weighting scheme, and the optimization method.

PEST ran the entire simulation (13 years) as many times as necessary to minimize the weighted sum of square within a specified tolerance. In some cases, a complete calibration run took 7 days, running on a laptop with 2.1GHz Intel Pentium Dual Core Processor and 4GB Memory.

CHAPTER SIX

MODEL EXPERIMENTS AND RESULTS

In the whole study process, 15 runs of PEST, numbered V2 through V16, were carried out to calibrate the Shenandoah model. In this chapter, four featured versions are described and discussed in detail. Related study results are described in order of time (the study procedure). Full records of the 15 trials are documented in ICPRB Shenandoah Watershed Modeling Report in Appendix B.

6.1 SWAT-PEST MODEL OUTPUT VERSION 2

In this very first version of iSWAT-PEST model, only surface runoff coefficient SURLAG, the roughness coefficients for main channels $n2_$, and the roughness coefficients for tributary channels $n1_$ were auto-calibrated by PEST. All other parameters were set to default values. The groundwater alpha parameter α for all soil types were set 0.048 according to previous work done by the ICPRB team. The groundwater beta parameter β for all soil types are set to 1, which represents a linear reservoir algorithm. Initial guesses of all other parameter values were determined from previous work by the ICPRB team. The weights for each observation group were set equally to 1, as described in Section 5.2. The $n2_$ values for main channels are in the .rte file; the $n1_$ values for tributary channels are in the .sub files.

PEST carried out three iterations. The original values and the final values for the parameters are recorded in Table 6.1.

Although the modeling period for iSWAT is from Nov. 1, 1994, to Oct. 31, 2006, the *R* and NSE are calculated for the model evaluation period, from Nov. 1, 1996, to Oct. 3, 2006. The reason is to eliminate the warm up period (Section 4.4).

Unfortunately, USGS gaging station at Christians Creek near Fishersville (observations for reach 10) discontinued in 1997. Therefore, the *R* and NSE for reach 10 are calculated from Nov. 1, 1995, to Sep. 17, 1997 (one-year warm-up period). Due to the effects of the warm-up period and short simulation time, statistics for reach 10 do not have much value and should not be taken into account in evaluating performances. Reach 10 will not be discussed in later sections. However, the statistics are still listed for reference and comparison purpose.

Table 6.1 Parameter Values in V2

Para.	Initial	Final
surlag	2.000	1.997
n1_sss	0.070	0.067
n1_lim	0.070	0.090
n1_lss	0.070	0.084
n1_col	0.070	0.075
n1_san	0.070	0.025
n2_sss	0.070	0.072
n2_lim	0.070	0.074
n2_lss	0.070	0.065
n2_col	0.070	0.071
n2_san	0.070	0.025

The Nash- Sutcliffe coefficients for each reach and the overall correlation coefficient R are listed in Table 6.2. R_w is the PEST weighted correlation coefficient as discussed in section 5.2. R is the non-weighted correlation coefficient calculated in the standard way.

Four out of 15 reaches show negative NSE, indicating that the SWAT-modeled daily discharges are no better prediction than the average annual hydrograph for these four reaches.

Within the positive ones, all are under the threshold value of 0.5, indicating poor prediction. Therefore, although the correlation coefficient shows a fair goodness of fit, this iSWAT version is considered poor.

Table 6.2 Goodness of Fit Statistics in V2

	Reach	V2
NSE	1	0.2510
	4	-0.7322
	5	0.4437
	6	0.2462
	7	0.1792
	10	-0.5499
	11	0.2940
	12	0.2960
	13	0.1507
	15	0.0642
	18	-0.2622
	19	-0.3977
	21	0.2591
	22	0.1978
	24	0.4183
R_w		0.8259
R_w^2		0.6821
R		0.8364
R^2		0.6996

The best prediction is in Reach 5, and the worst prediction is in Reach 4. The hydrographs for these two reaches from 1996 to 2006 are shown in Figures 6.1 and 6.2. Observing these hydrographs, two major problems exist in this version (circled in green). One problem is the generally low baseflow. This phenomenon shows not only in the poorly-performing reaches, but in the whole study area.

Possible reasons can be:

- 1) Groundwater parameters are fixed and set to the same value for all soil/geology type, which would incorrectly simulate baseflow.
- 2) Improper initial estimation of Manning's roughness coefficients. This improper initial estimation may not lead the objective function to global optimum.
- 3) Improper estimation of the channel slopes. This may result in quick recession and make SWAT unable to hold the predictions to the observed low flow level.
- 4) SWAT model tends to give better predictions on high flow. This is the inherent characteristic of SWAT, which is originally designed for modeling response to land use change.
- 5) The Y-axis is in logarithmic scale, which tends to exaggerate the differences in low flow and minimize the differences in high flow.

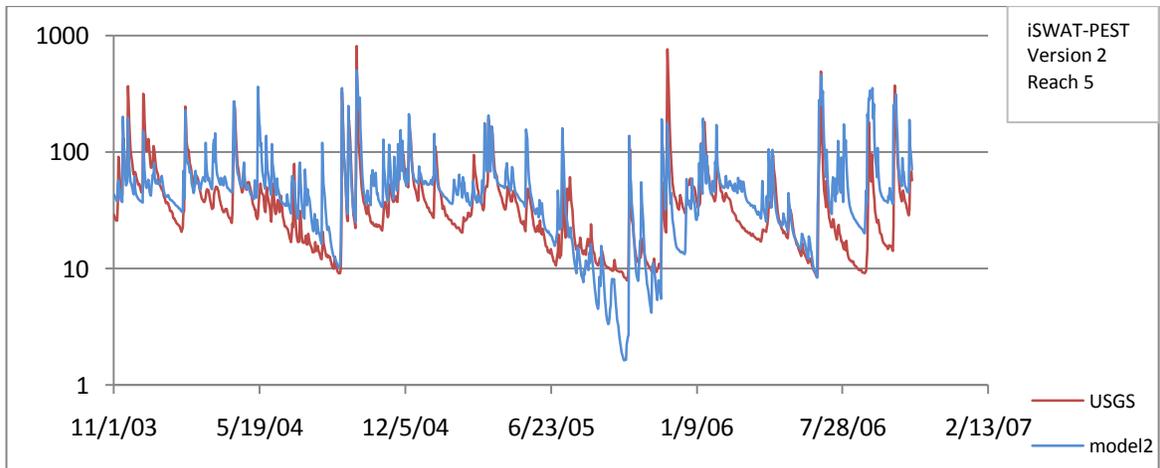
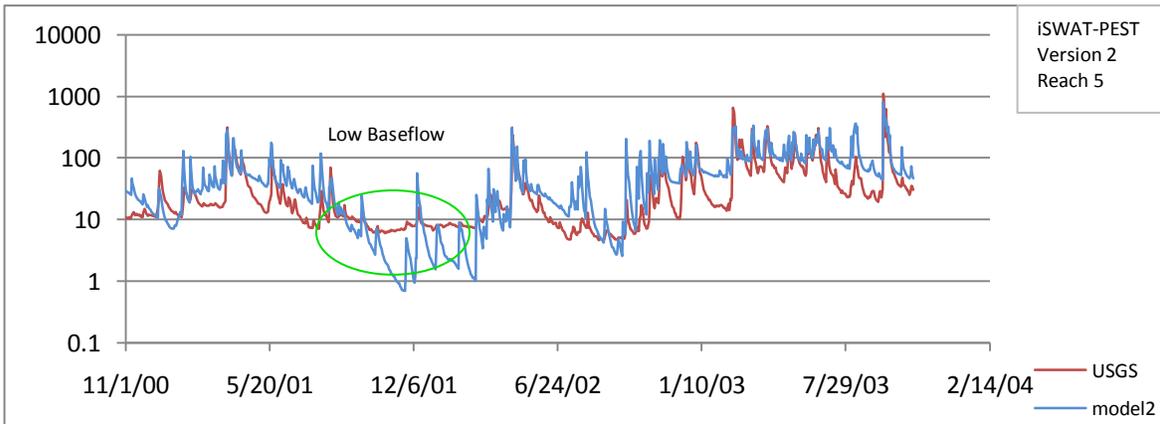
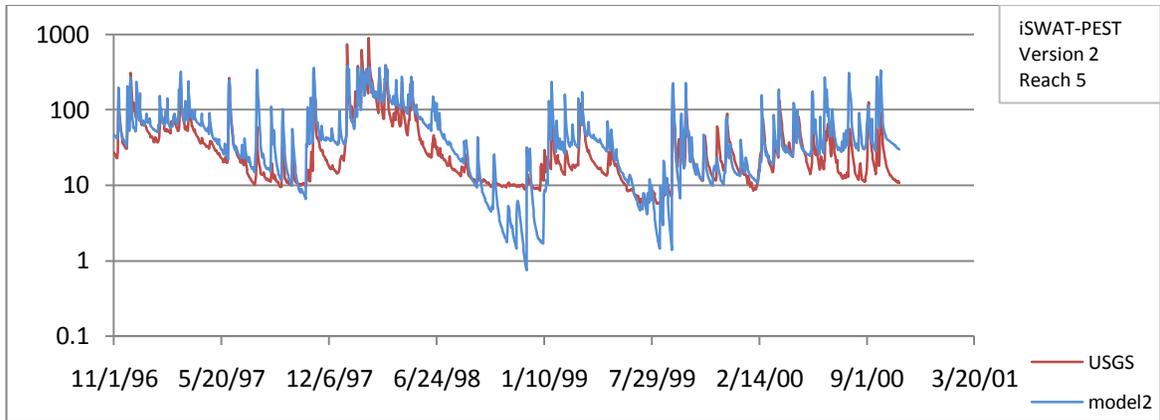


Figure 6.1 The Best Performing Reach in V2- Reach 5

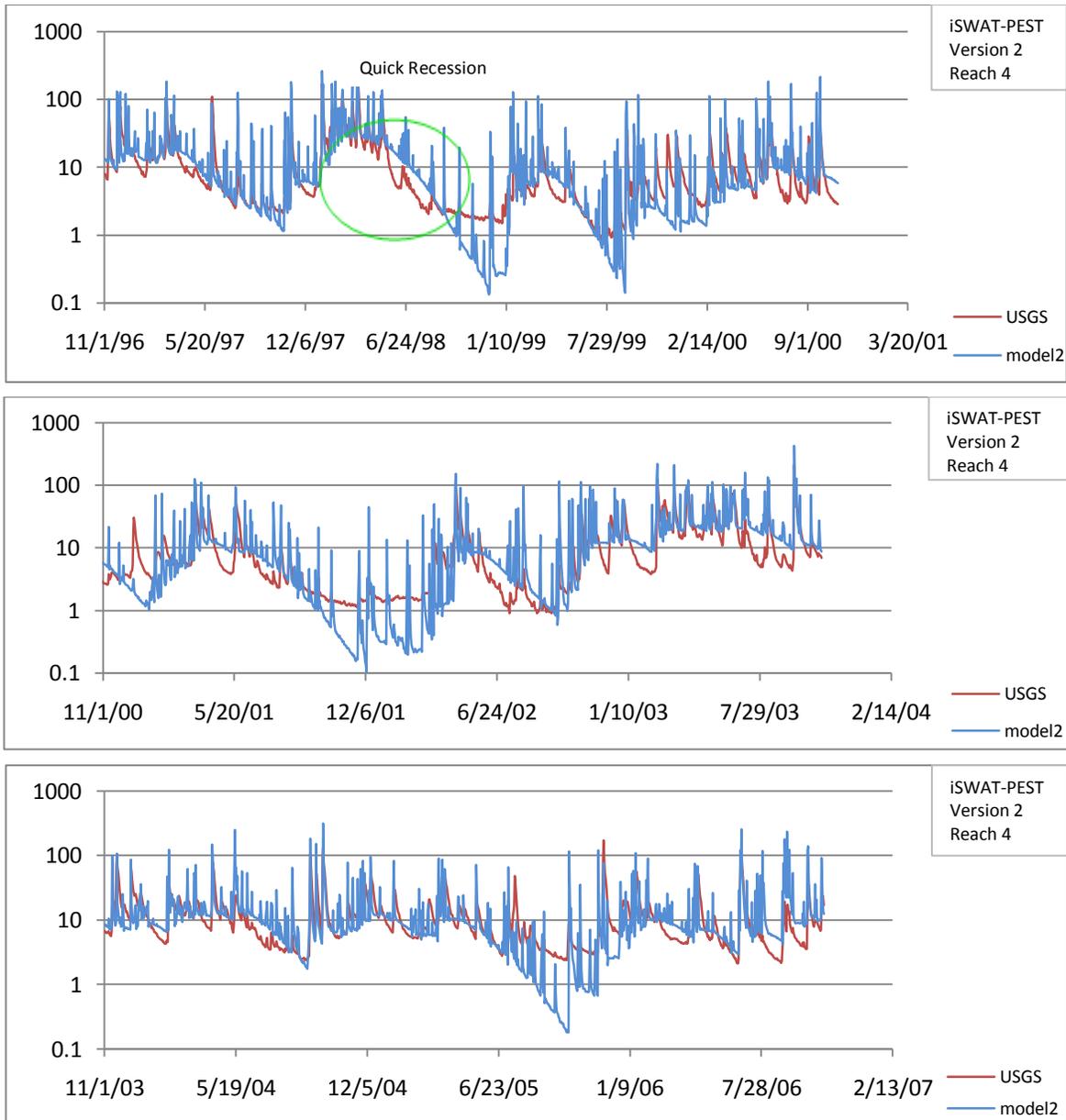


Figure 6.2 The Worst Performing Reach in V2- Reach 4

Another problem is quick recession. As one can observe from USGS hydrographs, discharge recession after each storm event is gentle and is concave in shape. However, the iSWAT modeled hydrographs show steep and convex trends. Moreover, the modeled recession time is generally greater than in real observations. The continuous recession worsens the low flow prediction.

Possible reasons can be:

- 1) Groundwater delay parameters are set too small. Increased delay time would smooth recession.
- 2) Bad estimation of low flow. Better low flow estimation would set proper lower bound for recession.

Based on all analysis above, from correlation coefficient to NSE, and to visual comparisons, this iSWAT version is considered a poor one.

6.2 iSWAT-PEST MODEL OUTPUT VERSION 3 MODIFIED

According to different soil types in each HRU, three groundwater related parameters, subsurface flow lengths, and soil evaporation parameters were introduced into the model. Moreover, according to different vegetation type (grossly divided into forest and crop), evapotranspiration parameters are also introduced. All $gd_$, $a_$, and $b_$ parameters are in .gwi files; $e_$, $s_$, can and $epco$ parameters are in .hru files.

This iSWAT-PEST version 3 still employs the equal-weighting method. All observations are given the same weights of 1. The PEST optimization performed 20 iterations, changing the parameter values into the final ones listed in Table 6.3.

The Nash- Sutcliffe coefficients for each reach and the overall correlation coefficient R are listed in Table 6.4. Results from V2 are included for comparison. Mean Discharges are also included for later discussion.

Having included more parameters, iSWAT-PEST Version 3m performed much better than version 2. NSEs for all 15 reaches improved dramatically. NSEs for all the reaches are now positive, except for reach 10, the one with

incomplete observation data. Four out of fifteen reaches can be considered fair prediction ($NSE > 0.5$). Two reaches' NSE are approximately 0.5.

R^2 also increases by 0.05, higher than the threshold value of 0.03 (An increasing of 0.03 for R^2 value is considered significant in improving model performance (McCuen, 2010)). Generally speaking, V3m greatly improves the model predictions by including parameters for baseflow and evapotranspiration.

Table 6.3 Parameter Values in V3m

Para.	Initial	Final	Para.	Initial	Final	Para.	Initial	Final
surlag	1.988	2.294	gd_sss	1.099	2.089	eva001	0.950	0.678
			gd_lim	1.968	0.043	eva002	0.950	0.591
n1_sss	0.070	0.060	gd_qua	1.000	1.000	eva003	0.950	0.709
n1_lim	0.070	0.124	gd_lass	1.035	0.710	eva004	0.950	0.718
n1_lass	0.065	0.025	gd_col	0.664	0.706	eva005	0.940	0.442
n1_col	0.071	0.050	gd_san	0.200	1.392	eva006	0.940	0.324
n1_san	0.070	0.075	gd_cry	1.503	0.086	eva016	1.000	0.063
						eva066	0.970	0.719
n2_sss	0.071	0.071	a_sss	0.002	0.005	eva069	0.970	0.962
n2_lim	0.070	0.079	a_lim	0.002	0.002	ewv114	0.900	0.900
n2_lass	0.070	0.075	a_qua	0.002	0.002			
n2_col	0.071	0.070	a_lass	0.002	0.005	sva001	51.000	76.882
n2_san	0.070	0.075	a_col	0.002	0.006	sva002	51.000	16.744
			a_san	0.002	0.001	sva003	41.000	60.016
cepco	0.990	0.585	a_cry	0.002	0.002	sva004	55.000	48.760
feeco	0.941	0.756				sva005	50.000	42.035
ccan	0.499	0.189	b_sss	0.535	0.624	sva006	50.000	41.928
fcan	0.501	0.494	b_lim	0.486	0.392	sva016	58.000	87.536
			b_qua	0.500	0.500	sva066	48.000	20.184
			b_lass	0.459	0.468	sva069	49.000	5.365
			b_col	0.502	0.483	swv114	50.000	50.000
			b_san	0.476	0.543			
			b_cry	0.522	0.496			

When comparing to the average discharge for each reach, one can observe a trend that higher average discharge is associated with higher NSE value.

Although it is not exactly true for all reaches, large rivers with more water flow such as reach 1 and 24 do have better predictions. This reflects the problem with equal weights--- PEST tends to focus more on large observations.

Table 6.4 Goodness of Fit Statistics in V3m

	Reach	V2	V3	Mean Discharge(cfs)
NSE	1	0.2510	0.6040	45.76
	4	-0.7322	0.2244	11.32
	5	0.4437	0.6311	40.87
	6	0.2462	0.5995	29.88
	7	0.1792	0.4887	9.12
	10	-0.5499	-0.4326	2.20
	11	0.2940	0.4188	7.29
	12	0.2960	0.3864	4.43
	13	0.1507	0.2284	2.91
	15	0.0642	0.4577	18.16
	18	-0.2622	0.2982	2.26
	19	-0.3977	0.2227	5.60
	21	0.2591	0.3867	1.09
	22	0.1978	0.3854	2.17
24	0.4183	0.6560	83.79	
R_w		0.8259	0.8557	
R_w^2		0.6821	0.7322	
R		0.8364	0.8634	
R^2		0.6996	0.7455	

Hydrographs for the worst performing reach 19 are shown in Figure 6.3.

Although the baseflow condition has been improved, relative to V2, it is actually over-adjusted. The previous under-predicted low flow is now over-predicted. It seems that PEST tried to minimize the overall variance, thus increasing low flows and decreasing high flows. Another problem shown here is noise in the model. The model output is not as smooth as the observations.

Generally speaking, iSWAT-PEST Version 3 is a fair model. It is an improvement over the previous version.

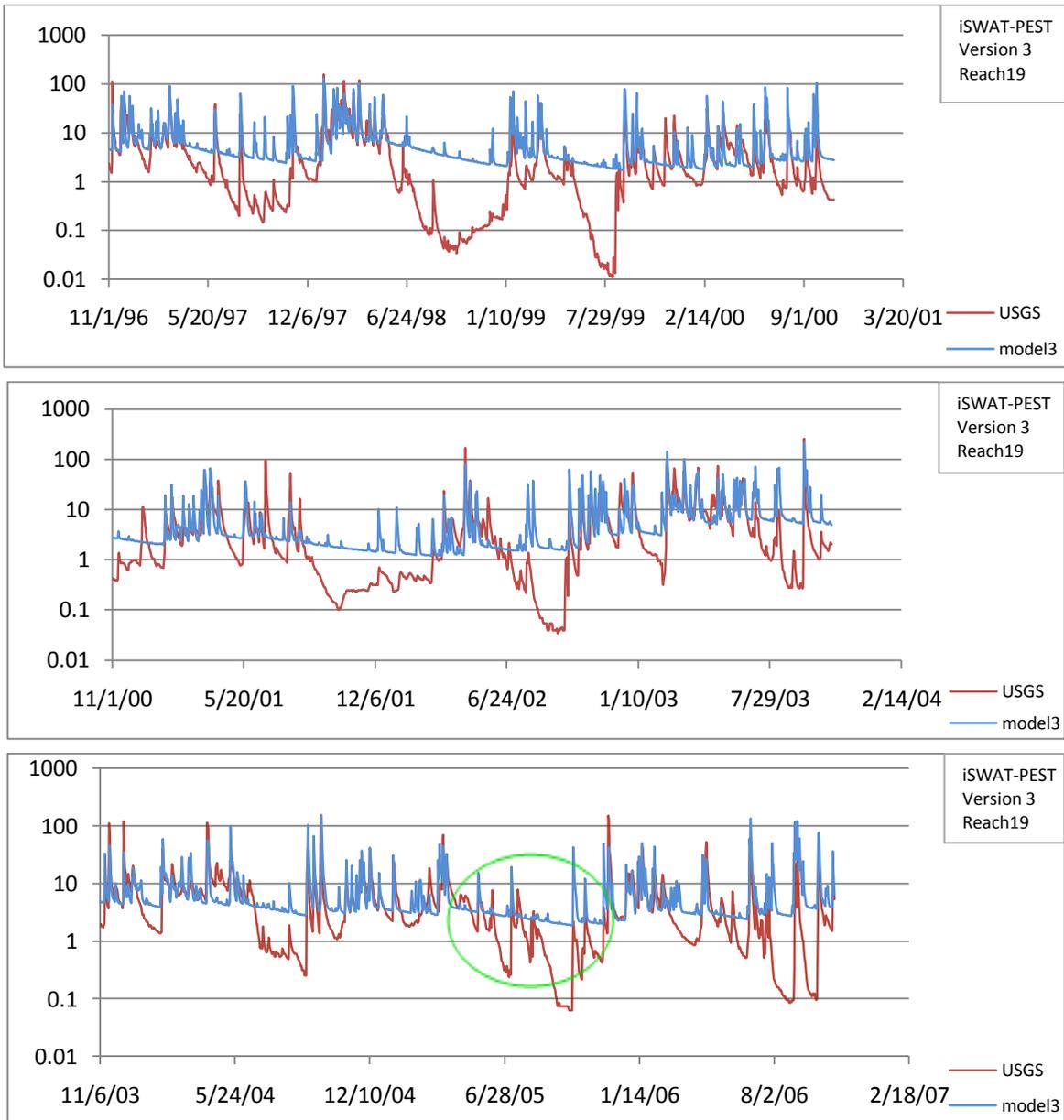


Figure 6.3 The Worst Performing Reach in V3m – Reach 19

6.3 iSWAT-PEST MODEL OUTPUT VERSION 9

Some changes are made in this version. First, the ordinal weighting method is employed. Second, the roughness coefficient parameters for the tributary channels are modified.

The Manning's n values for the tributary channels were previously assigned by the soil type dominant the main channel. However, it is considered improper to use the main channel soil type to determine the tributary soil type. Therefore, the Manning's n values for the tributary channels were re-evaluated on the basis of dominant soil type in the subwatershed.

To achieve this, information about soil type and the area fraction of each HRU in the whole subwatershed should first be collected. Then the dominant soil type was determined by choosing the soil type which has the highest percentage-coverage of the subwatershed. If two types of soil have similar shares, the dominant one was determined by examining the physical location and soil map of the stream network.

By reclassifying the dominant soil type for tributaries, a new parameter "n1_cry" was added in the PEST control file and template files, corresponding to crystalline geology and its associated soil. Also in .ptf files, most subbasins were assigned a different n1 parameter (ex. changed from n1_lim to n1_san) because the dominant soil type in the entire subbasin differs from the soil surrounding the main stream reach. Table 6.5 lists the new n1 parameters. Red letters indicate a change in n1 type.

Table 6.5 New Roughness Coefficients Designation

Subbasin	Soil fraction	New n1	Old n1
0501	0.457	n1_cry	n1_col
0502	0.609	n1_san	n1_col
0503	0.519	n1_san	n1_col
0504	0.584	n1_lass	n1_col
0505	0.461	n1_san	n1_col
0506	0.609	n1_lass	n1_col
0507	0.451	n1_lass	n1_col
0508	0.995	n1_lass	n1_lass
0509	0.591	n1_lass	n1_lass
0510	0.766	n1_lass	n1_sss
0511	0.429	n1_col	n1_col
0512	0.500	n1_col	n1_col
0601	0.546	n1_sss	n1_sss
0602	0.704	n1_lim	n1_lim
0603	0.519	n1_lim	n1_sss
0604	0.290	n1_sss	n1_col
0605	0.494	n1_san	n1_sss
0606	0.677	n1_san	n1_sss
0607	0.716	n1_sss	n1_col
0608	0.772	n1_lass	n1_col
0609	0.623	n1_lim	n1_lim
0610	0.323	n1_san	n1_lim
0701	0.743	n1_lim	n1_san
0702	0.713	n1_lim	n1_col
0703	0.570	n1_lim	n1_col
0704	0.453	n1_lim	n1_col
0705	0.404	n1_cry	n1_col
0706	0.690	n1_sss	n1_lim

PEST performed a total of 6 optimization iterations, changing the parameter values into the final ones listed in Table 6.6.

The Nash- Sutcliffe Coefficients for each reach and the correlation coefficient R are listed in Table 6.7. Previous results are also included for comparison.

Table 6.6 Parameter Values in V9

Para.	Initial	Final
surlag	1.6220	2.0017
n1_cry	0.0500	0.0250
n1_sss	0.1500	0.0283
n1_lim	0.0276	0.0250
n1_lss	0.0540	0.0259
n1_col	0.0731	0.0777
n1_san	0.1250	0.0647
n2_sss	0.0745	0.0739
n2_lim	0.0701	0.0765
n2_lss	0.0657	0.0695
n2_col	0.0708	0.0717
n2_san	0.1250	0.1250
cepco	0.9900	0.9693
fepco	0.9410	0.9206
ccan	0.4990	0.5460
fcan	0.5010	0.5177

Para.	Initial	Final
gd_sss	1.1711	1.6165
gd_lim	0.0250	0.0250
gd_qua	1.0000	1.0000
gd_lss	4.3833	1.5968
gd_col	1.2571	0.8813
gd_san	2.6570	4.3992
gd_cry	0.3057	0.0223
a_sss	0.0139	0.0167
a_lim	0.0003	0.0003
a_qua	0.0020	0.0020
a_lss	0.0044	0.0081
a_col	0.0050	0.0057
a_san	0.0010	0.0009
a_cry	0.0002	0.0003
b_sss	0.9852	1.0000
b_lim	0.1442	0.1583
b_qua	0.5000	0.5000
b_lss	0.5131	0.4864
b_col	0.6535	0.5782
b_san	0.1000	0.1702
b_cry	0.4484	0.4290

Para.	Initial	Final
eva001	0.9500	0.7702
eva002	0.9500	0.8319
eva003	0.9500	0.8664
eva004	0.9500	0.6356
eva005	0.9400	0.6475
eva006	0.9400	0.8814
eva016	1.0000	0.3533
eva066	0.9700	0.9272
eva069	0.9700	1.0000
ewv114	0.9000	0.9000
sva001	51.0000	90.0000
sva002	51.0000	35.4055
sva003	41.0000	59.4663
sva004	55.0000	49.4169
sva005	50.0000	64.2221
sva006	50.0000	42.2098
sva016	58.0000	57.4508
sva066	48.0000	35.7923
sva069	49.0000	47.8940
swv114	50.0000	50.0000

In this version, the Correlation Coefficient changes, as does the NSE for each reach. R^2 decreases 0.045 to a value of 0.6874. Although the number doesn't exceed 0.7, the rule of thumb for good prediction, 0.687 is approximately the same as 0.7. Therefore, this model would still be considered as a good prediction in consideration of R^2 .

The 15 NSEs stays about the same for most reaches, changing less than 0.02. NSEs increase for reaches 4, 6, 11, 12, 15, 18, 22; decrease for reaches 7,

13 and 21. Four reaches can be considered as fair prediction. 3 reaches' NSE are approximately 0.5.

Table 6.7 Goodness of Fit Statistics in V9

	Reach	V2	V3m	V9
NSE	1	0.2510	0.6040	0.5867
	4	-0.7322	0.2244	0.3870
	5	0.4437	0.6311	0.6284
	6	0.2462	0.5995	0.6135
	7	0.1792	0.4887	0.3802
	10	-0.5499	-0.4326	-0.8047
	11	0.2940	0.4188	0.4686
	12	0.2960	0.3864	0.4473
	13	0.1507	0.2284	0.1681
	15	0.0642	0.4577	0.4708
	18	-0.2622	0.2982	0.3100
	19	-0.3977	0.2227	0.1993
	21	0.2591	0.3867	0.2811
	22	0.1978	0.3854	0.4131
24	0.4183	0.6560	0.6387	
R_w		0.8259	0.8557	0.8291
R_w^2		0.6821	0.7322	0.6874
R		0.8364	0.8634254	0.8593
R^2		0.6996	0.7455	0.7384

This version takes into account the tributaries and main reach within the whole watershed. The water from tributaries flows into the main ones and accumulates with flows from other tributaries. The previously poorly performing reach (4) now performs much better.

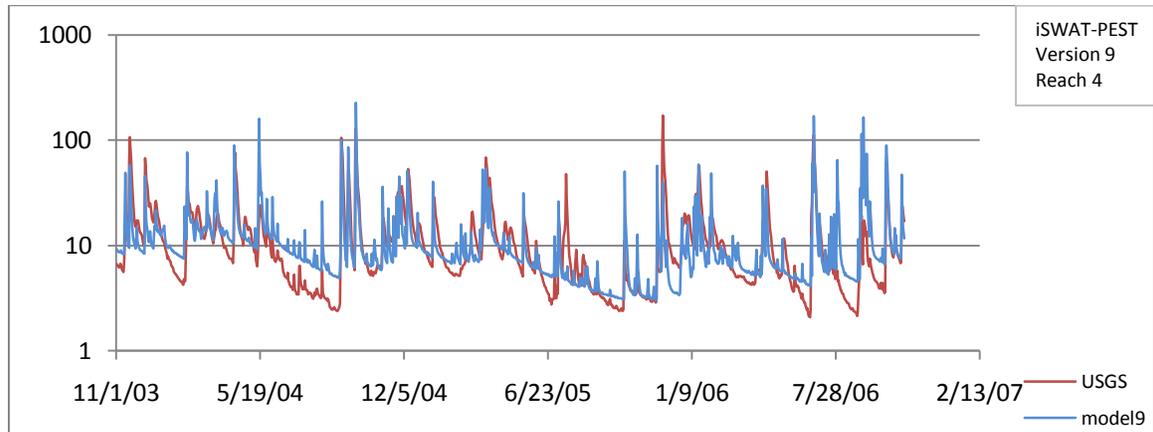
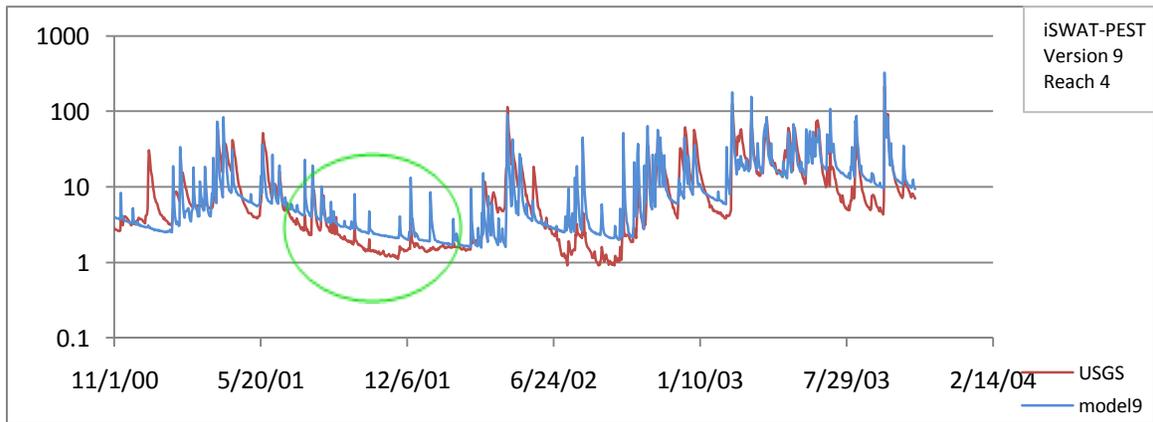
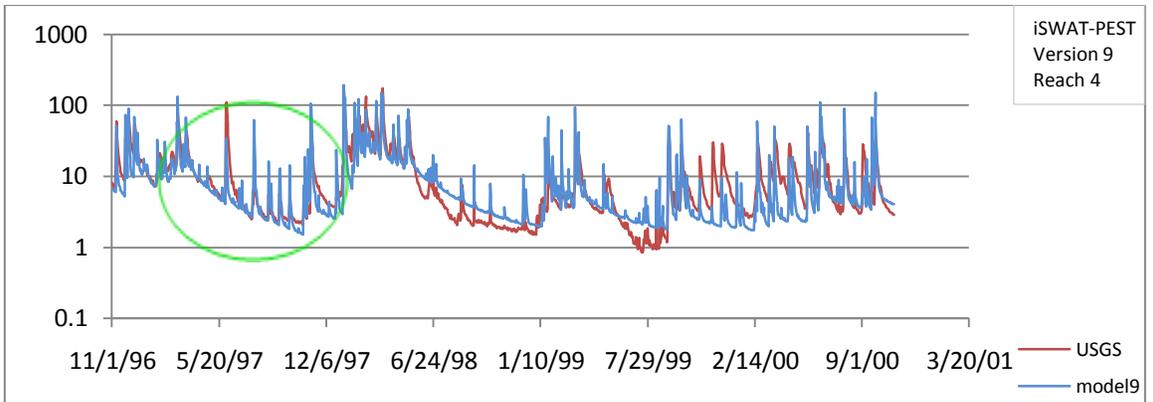


Figure 6.4 Hydrographs for Reach 4 in V9

In Figure 6.4, see some closely matched recessions are visible. Also, the base flow (low flow) is improved. Therefore, although the statistics stay the same or even worse for certain reaches, the overall performances of this version improves in sense of recession and base flow prediction.

6.4 NEW ROUGHNESS COEFFICIENTS FOR MAIN CHANNELS

As described in section 5.4. Empirical equations and GIS were used to recalculate the roughness coefficients for the main channels, instead of making them adjustable in auto-calibration. The results are shown in Table 6.8.

Table 6.8 New Roughness Coefficients for Each Subbasin

subbasin	n_new_GIS	n2_soil	n2 parameters	Original n2 values
0501	0.0338	VA004	n2_col	0.07135
0502	0.0607	VA004	n2_col	0.07135
0503	0.0422	VA004	n2_col	0.07135
0504	0.0377	VA004	n2_col	0.07135
0505	0.0215	VA004	n2_col	0.07135
0506	0.0209	VA004	n2_col	0.07135
0507	0.0218	VA004	n2_col	0.07135
0508	0.0242	VA003	n2_lass	0.06687
0509	0.0418	VA003	n2_lass	0.06687
0510	0.0502	VA066	n2_sss	0.07446
0511	0.0244	VA004	n2_col	0.07135
0512	0.0412	VA004	n2_col	0.07135
0601	0.0592	VA066	n2_sss	0.07446
0602	0.0305	VA002	n2_lim	0.06733
0603	0.0208	VA066	n2_sss	0.07446
0604	0.0210	VA004	n2_col	0.07135
0605	0.0573	VA066	n2_sss	0.07446
0606	0.0593	VA066	n2_sss	0.07446
0607	0.0639	VA004	n2_col	0.07135
0608	0.0402	VA004	n2_col	0.07135
0609	0.0439	VA002	n2_lim	0.06733
0610	0.0414	VA002	n2_lim	0.06733
0701	0.0214	VA005	n2_san	0.12500
0702	0.0158	VA004	n2_col	0.07135
0703	0.0139	VA004	n2_col	0.07135
0704	0.0122	VA004	n2_col	0.07135
0705	0.0123	VA004	n2_col	0.07135
0706	0.0249	VA002	n2_lim	0.06733

The first column shows the code for each sub-watershed. The second column shows the modified roughness coefficients for main channels. The third column is the dominant soil type along the main channel. The fourth column is the

parameter originally assigned in the model. The last column lists the n_2 values as determined by auto-calibration in V9.

There is actually no pattern in n values by soil type. It shows that even if the soil type surrounding the main channel is the same in two subbasins, the roughness coefficients may differ due to the physical characteristics of the drainage areas (reach length, relief, etc.).

6.5 iSWAT-PEST MODEL OUTPUT VERSION 16

In this iSWAT-PEST version, the new roughness coefficients for main channels are assigned to each subbasin based on McCandless (2003) and GIS analysis (chapter 5.3). In the PEST control file, these n_2 parameters are set fixed, which means they are not allowed to change in the calibration process.

Also in the SWAT input files and PEST template files, the main channel lengths and slope, and the subbasin areas are modified into the GIS calculated ones (for detailed differences, refer to chapter 5.3)

PEST performed 23 optimization iterations, changing the parameter values into the final ones listed in Table 6.9. The n_2 values are fixed, so they are not documented here. For detailed n_2 value, see chapter 5.3 3).

During these 23 iterations, PEST actively explored the parameter space to identify the best parameter set. The parameter changes over each iteration are shown in Figures 6.5.

Table 6.9 Parameter Value in V16

Para.	Initial	Final
surlag	1.3540	0.8620
n1_cry	0.0250	0.0250
n1_sss	0.0714	0.0250
n1_lim	0.0278	0.0250
n1_lass	0.0729	0.0250
n1_col	0.1148	0.0618
n1_san	0.0548	0.0362
cepc0	0.9900	0.4041
fepco	0.9410	0.8017
ccan	0.4990	0.4192
fcan	0.5010	0.6014

Para.	Initial	Final
gd_sss	1.1711	0.6501
gd_lim	0.0010	0.0010
gd_qua	0.0010	0.0010
gd_lass	4.3833	2.0951
gd_col	1.2571	0.7855
gd_san	2.6570	0.0521
gd_cry	0.3057	0.4391
a_sss	0.0139	0.0131
a_lim	0.0003	0.0004
a_qua	0.0001	0.0001
a_lass	0.0044	0.0081
a_col	0.0050	0.0445
a_san	0.0010	0.0014
a_cry	0.0002	0.0005
b_sss	0.9852	0.4261
b_lim	0.1442	0.3803
b_qua	0.1000	0.1286
b_lass	0.5131	0.3961
b_col	0.6535	0.2753
b_san	0.1000	0.4490
b_cry	0.4484	0.9312

Para.	Initial	Final
eva001	0.9500	0.3106
eva002	0.9500	0.0545
eva003	0.9500	0.8307
eva004	0.9500	0.1513
eva005	0.9400	0.0964
eva006	0.9400	0.4534
eva016	1.0000	0.0100
eva066	0.9700	0.9869
eva069	0.9700	1.0000
ewv114	0.9000	0.9000
sva001	51.0000	90.0000
sva002	51.0000	31.0104
sva003	41.0000	49.4542
sva004	55.0000	12.3501
sva005	50.0000	90.0000
sva006	50.0000	68.4122
sva016	58.0000	25.4688
sva066	48.0000	60.7931
sva069	49.0000	2.2063
swv114	50.0000	50.0000

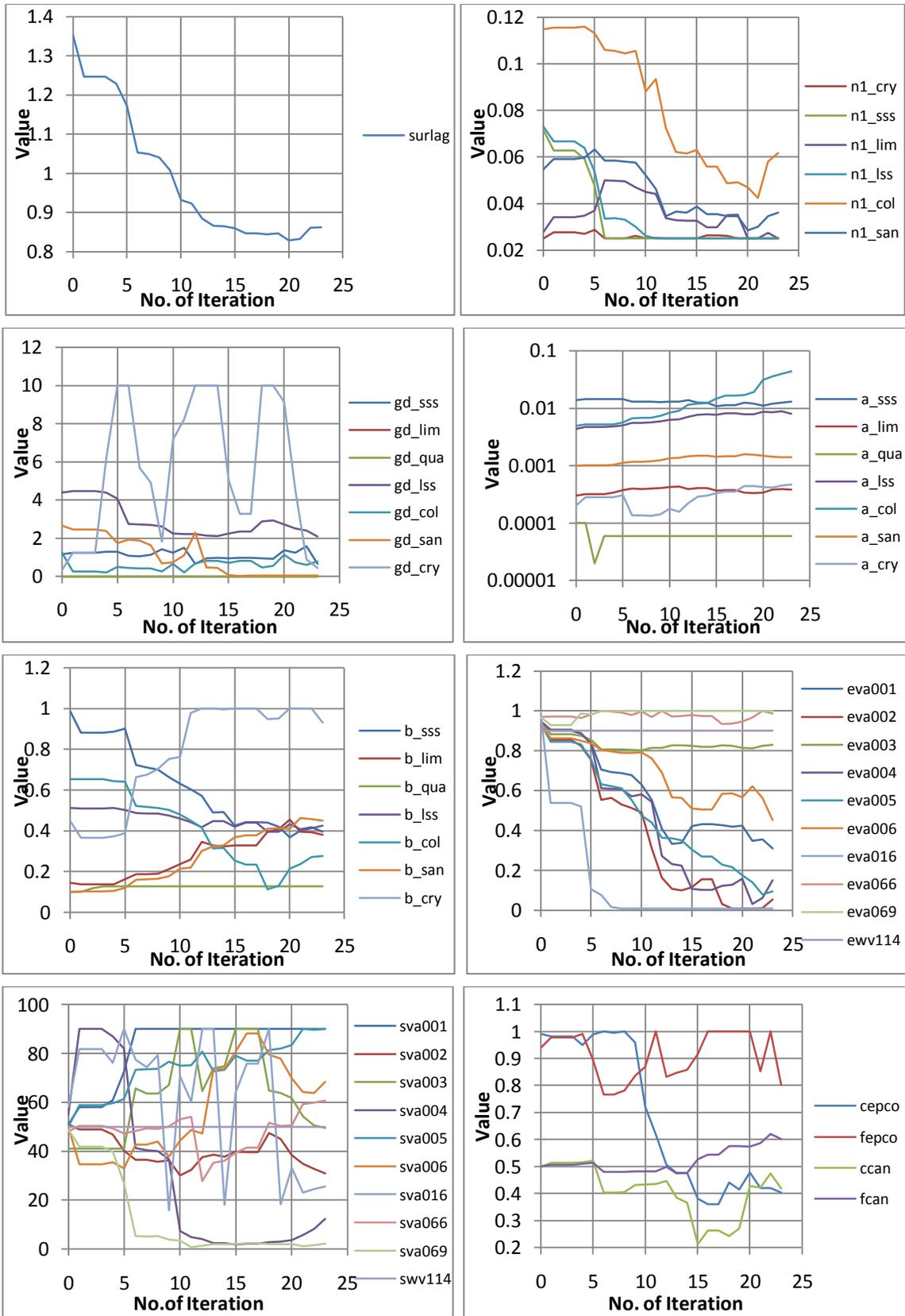


Figure 6.5 Parameter Changes in Each Iteration in V16

The Nash- Sutcliffe Coefficients for each reach and the correlation coefficient R are provided in Table 6.10, together with previous results for comparison.

Table 6.10 Goodness of Fit Statistics for V16

	Reach	V2	V3m	V9	V16
NSE	1	0.2510	0.6040	0.5867	0.5650
	4	-0.7322	0.2244	0.3870	0.5959
	5	0.4437	0.6311	0.6284	0.6887
	6	0.2462	0.5995	0.6135	0.7064
	7	0.1792	0.4887	0.3802	0.3873
	10	-0.5499	-0.4326	-0.8047	-0.1724
	11	0.2940	0.4188	0.4686	0.5001
	12	0.2960	0.3864	0.4473	0.4446
	13	0.1507	0.2284	0.1681	0.3140
	15	0.0642	0.4577	0.4708	0.4824
	18	-0.2622	0.2982	0.3100	0.4541
	19	-0.3977	0.2227	0.1993	0.3681
	21	0.2591	0.3867	0.2811	0.4097
	22	0.1978	0.3854	0.4131	0.5173
24	0.4183	0.6560	0.6387	0.4816	
R_w		0.8259	0.8557	0.8291	0.8293
R_w^2		0.6821	0.7322	0.6874	0.6877
R		0.8364	0.8634	0.8593	0.8392
R^2		0.6996	0.7455	0.7384	0.7043

In this very last version of iSWAT-PEST, the overall correlation coefficient doesn't change much, keep $R^2 = 0.7$ approximately. However, the NSEs for all the reaches increase a lot. 6 reaches can be considered as fair prediction. 4 reaches' NSE are approximately 0.5. All NSEs are above 0.3, and this can be considered as an improvement for the whole watershed model.

The hydrographs for the previously mentioned 4 reaches, Reach 4, 5, 19 and the final outlet on Reach 24 are shown below. Improvement can be observed clearly.

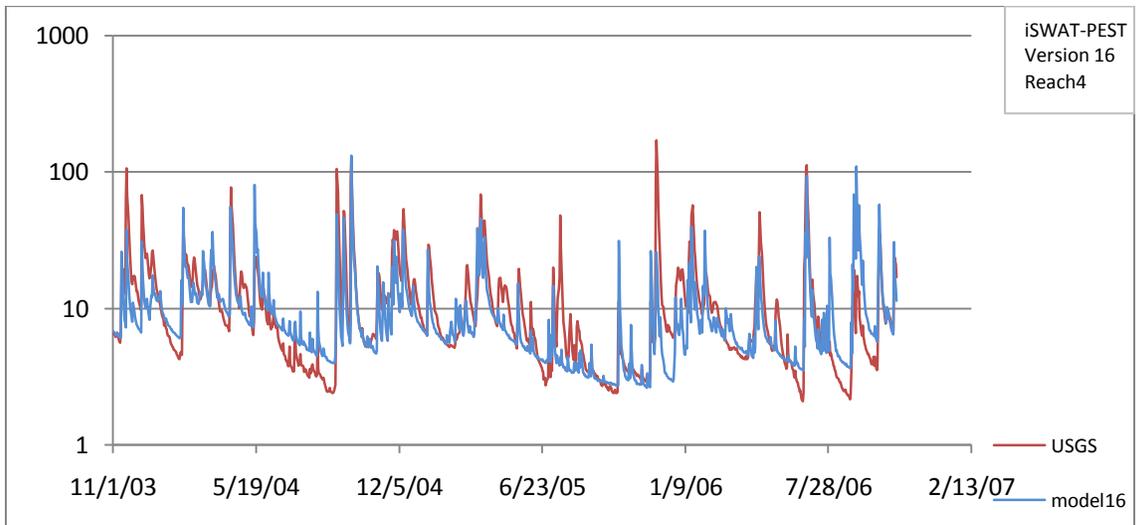
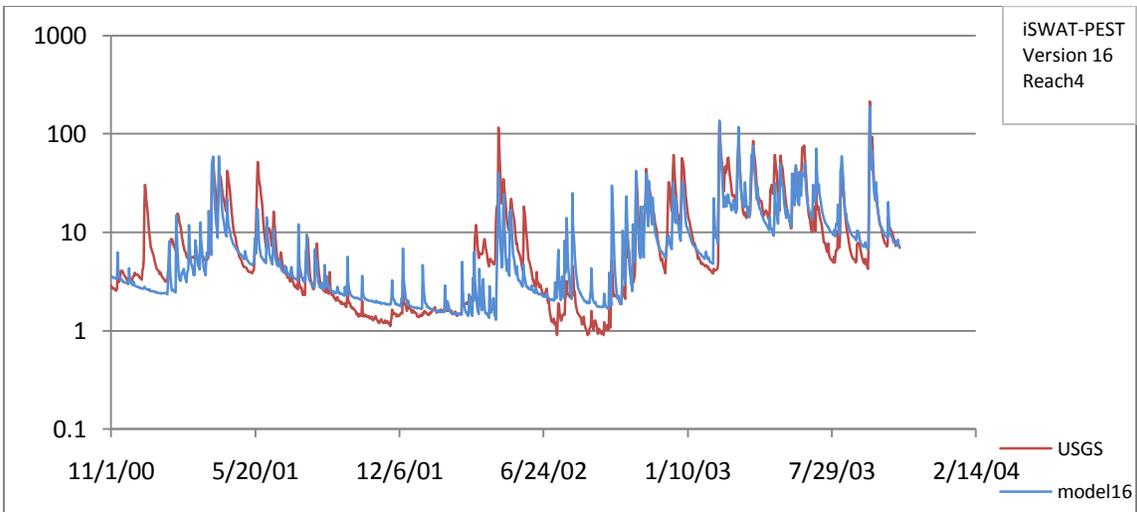
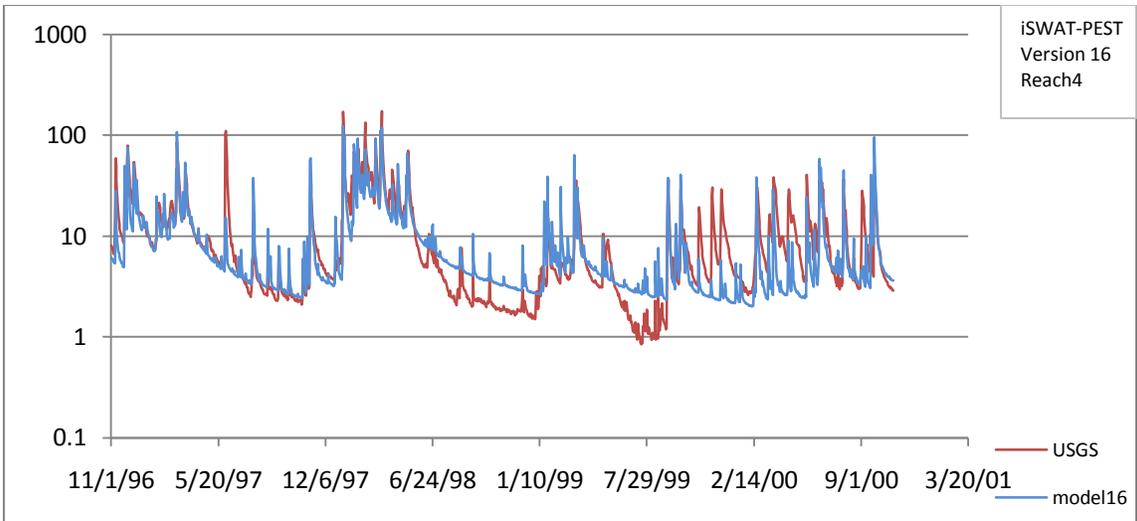


Figure 6.6 Hydrographs for Reach 4 in V16

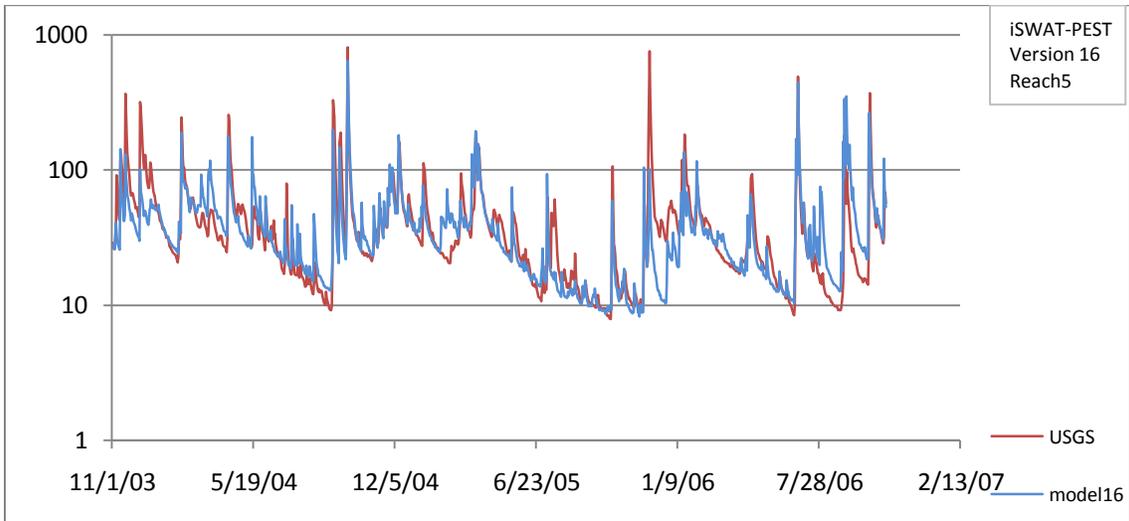
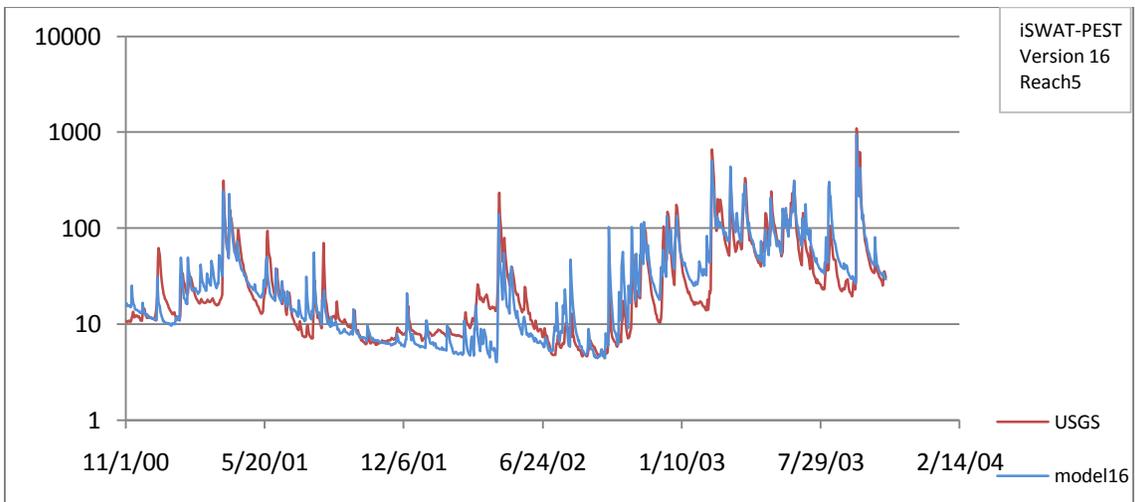
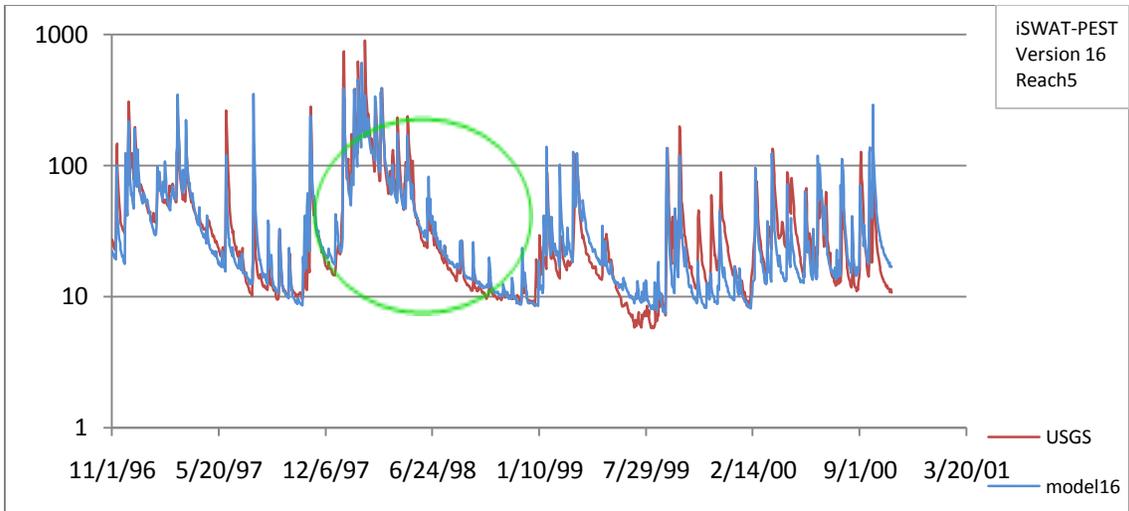


Figure 6.7 Hydrographs for Reach 5 in V16

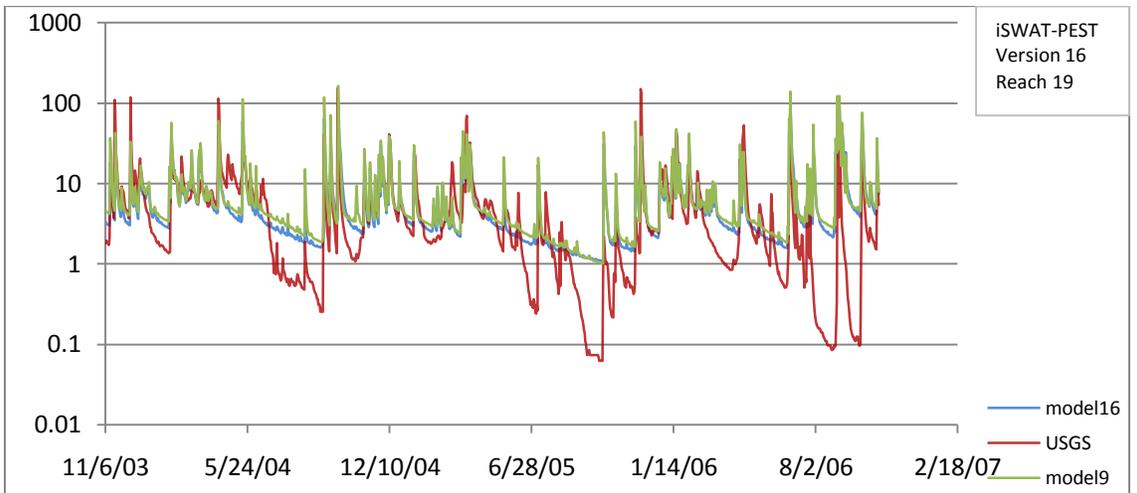
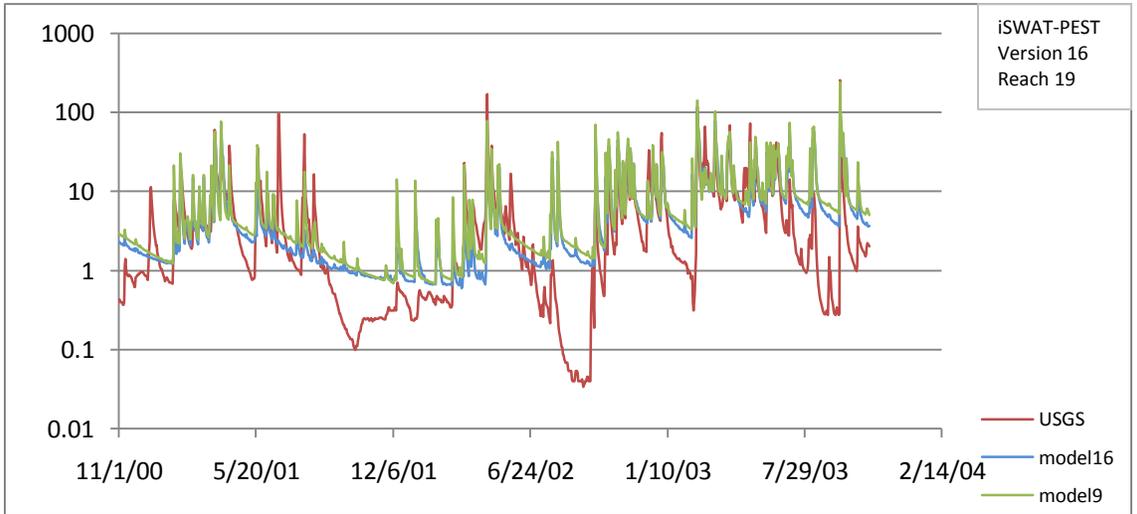
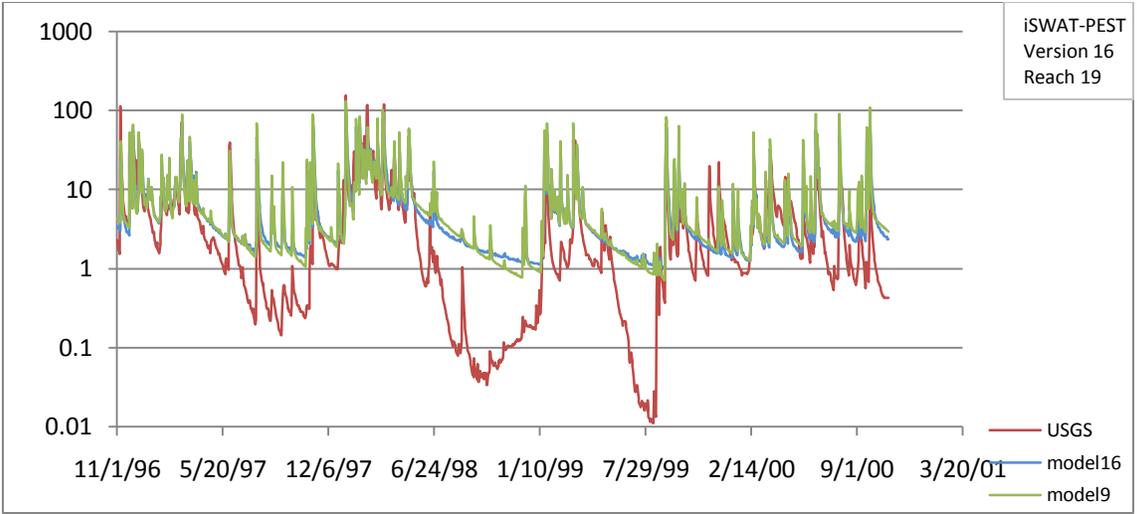


Figure 6.8 Hydrographs for Reach 19 in V16

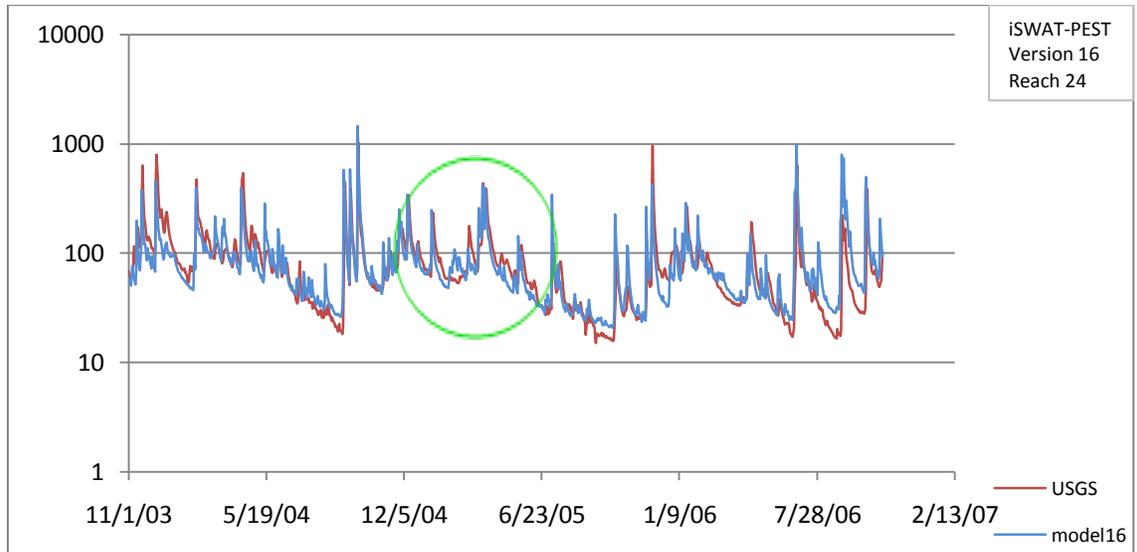
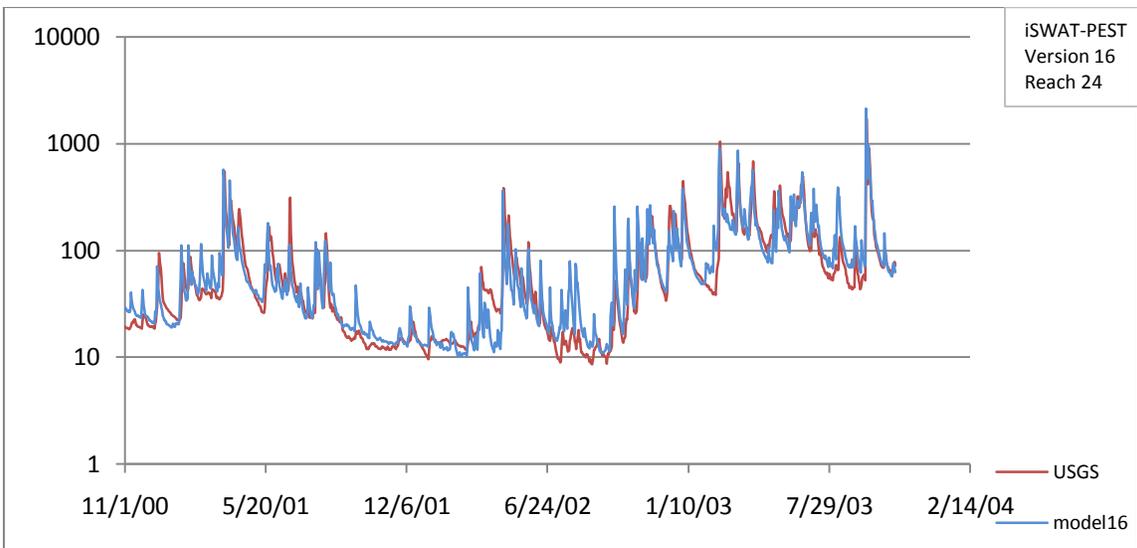
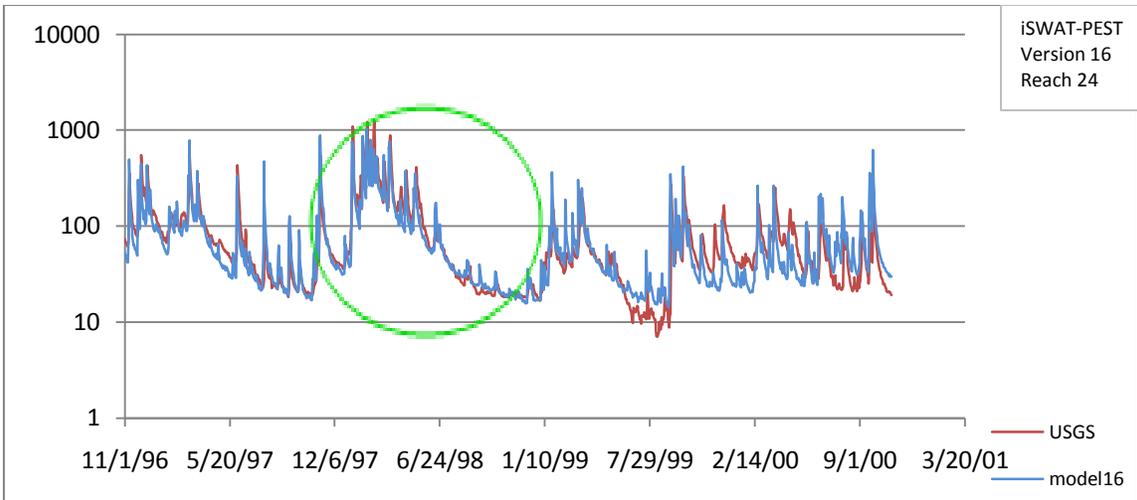


Figure 6.9 Hydrographs for Reach 24 in V16

In reach 19, the result from version 9 was included to compare with the result from version 16. Although SWAT still doesn't perform well in both versions, V16 performs slightly better than V9: recessions are smoother and low flow closer to observations.

One can compare reach 4, reach 5 and reach 24 to the outputs from other versions, there are big improvements and the modeled hydrographs match well with observed ones.

For the 11-year period of observation, a total of $306007 \times 60 \times 60 \times 24 \text{ m}^3$ of water ran through the gaging station at reach 24. Version 16 modeled a total of $298865 \times 60 \times 60 \times 24 \text{ m}^3$ of water for reach 24. The underprediction only accounts for 2.3% of total water quantity. Below is a record of other previously mentioned versions in aspect of total water flow. Improvements are seen from each later version.

Table 6.11 Total Water Simulated for 11 Years in Each Version

USGS	V3	V9	V16
306007.42	331299.66	318391.13	298865.43
Difference	25292.24	12383.71	-7141.99
Diff. Fraction	0.0827	0.0405	-0.0233

As a conclusion, this iSWAT-PEST Version 16 does a good job in simulating the river discharge for the Shenandoah Valley Watershed.

6.6 EVALUATION OF PARAMETER RATIONALITY

To evaluate the parameter rationality, a brief sensitivity analysis was carried out. In this analysis, parameter set obtained from V16 was chosen the base

parameter set, to be compared to other parameter sets. In each comparison parameter set, only one of the adjustable parameters was modified (increased or decreased) by 10%. Most parameters were increased by 10% (subjectively assigned). However, if increasing the parameter value resulted in values over the parameter upper limit, this particular parameter was decreased by 10%. Note: the n2 values are not modified because these values were fixed to the calculated value from the empirical equations.

The total modeled discharge of the 13-year period for reach 24 from each comparison parameter set was then compared to that from the base set. The results are shown in Table 6.12.

Table 6.12 Parameter values in sensitivity analysis

	Original Values	parameter change	bias total	bias mean
surlag	0.861957	*1.1	18.22	0.0050
n1_cry	0.025	*0.9	15.56	0.0043
n1_sss	0.025	*0.9	1.75	0.0005
n1_lim	0.025	*0.9	7.63	0.0021
n1_lss	0.025	*0.9	1.24	0.0003
n1_col	0.061799	*0.9	3.82	0.0010
n1_san	0.036179	*0.9	6.70	0.0018
gd_sss	0.650089	*0.9	0.79	0.0002
gd_lim	0.001	*1.1	0.00	0.0000
gd_qua	0.001	*1.1	0.00	0.0000
gd_lss	2.09507	*1.1	3.55	0.0010
gd_col	0.785498	*1.1	2.17	0.0006
gd_san	0.052148	*1.1	0.00	0.0000
gd_cry	0.439132	*1.1	0.00	0.0000
a_sss	0.013131	*1.1	-1.73	-0.0005
a_lim	0.000386	*1.1	1290.13	0.3532
a_qua	6E-05	*1.1	0.00	0.0000
a_lss	0.008051	*1.1	-18.01	-0.0049
a_col	0.044474	*1.1	-0.87	-0.0002
a_san	0.001414	*1.1	977.32	0.2675
a_cry	0.000472	*1.1	339.19	0.0929

Table 6.12 Parameter values in sensitivity analysis (Con.)

b_sss	0.426115	*1.1	2.16	0.0006
b_lim	0.380316	*1.1	585.17	0.1602
b_qua	0.128608	*1.1	0.00	0.0000
b_iss	0.396136	*1.1	21.44	0.0059
b_col	0.275327	*1.1	3.82	0.0010
b_san	0.449038	*1.1	229.47	0.0628
b_cry	0.931239	*1.1	436.65	0.1195
eva001	0.310631	*1.1	191.58	0.0524
eva002	0.054541	*1.1	7.05	0.0019
eva003	0.830694	*1.1	8682.69	2.3769
eva004	0.151253	*1.1	36.55	0.0100
eva005	0.096403	*1.1	94.51	0.0259
eva006	0.453384	*1.1	453.17	0.1241
eva016	0.01	*0.9	0.22	0.0001
eva066	0.986946	*0.9	-1715.50	-0.4696
eva069	1	*1.1	-2541.88	-0.6958
ewv114	0.9	*1.1	0.00	0.0000
sva001	90	*1.1	-9.45	-0.0026
sva002	31.0104	*1.1	-92.30	-0.0253
sva003	49.4542	*1.1	-6.22	-0.0017
sva004	12.3501	*1.1	-5.97	-0.0016
sva005	90	*1.1	-76.32	-0.0209
sva006	68.4122	*1.1	-295.03	-0.0808
sva016	25.4688	*1.1	-1.99	-0.0005
sva066	60.7931	*1.1	-5.47	-0.0015
sva069	2.20629	*1.1	-224.75	-0.0615
swv114	50	*1.1	0.00	0.0000
cepco	0.404125	*1.1	-368.25	-0.1008
fepco	0.801673	*1.1	-68.63	-0.0188
ccan	0.4192	*1.1	-32.35	-0.0089
fcan	0.60141	*1.1	-189.36	-0.0518

The expected results and the modeled output are listed in Table 6.13. “√” means the modeled results agree with the expectations.

Table 6.13 Parameter Rationality: Model Results versus Expectations

Para.	Change	Expected results	Modeled results
surlag	increases	less water stored and more discharge	√
n1_	decreases	higher discharge	√
gd_	increases	no obvious expectation	√
a_	increases	higher baseflow; maybe higher discharge	
b_	increases	higher baseflow; maybe higher discharge	√
e_	increases	higher flow into river	√
s_	increases	higher evaporation; less discharge	√
_epco	increases	more water uptaken by plant; less discharge	√
_can	increases	more water stored on leaves; less discharge	√

The baseflow alpha parameter ($a_$) not only related to baseflow reaching the rivers, but also related to water recharge. Therefore, the effect of this parameter is hard to determine.

In conclusion, all the parameters are rational. The changes in these parameter values generate changes in output that are consistent with the physical processes they are intended to represent.

6.7 COMPARISON OF R AND R_w IN ALL MODEL VERSIONS

The non-weighted correlation coefficients R and the weighted correlation coefficients R_w are listed in Table 6.14.

According to Figure 6.10, overall R^2 increases when all adjustable parameters are include in Version 3m. R^2 decreases from Version 12 and increases again in Version 16. The weighted R_w^2 decreases dramatically in Version 5. However, it increases when new $n2$ values are included in the model in version 10. Though there is a slight drop in version 12, the value increases again in Version 16. Overall evaluation of the model shows that V16 performs best.

Table 6.14 R and R_w values in each version

	V2	V3	V3m	V4	V5	V6	V7	V8
R	0.8364	0.8091	0.8634	0.8212	0.8702	0.8632	0.8611	0.8696
R^2	0.6996	0.6546	0.7455	0.6744	0.7572	0.7450	0.7416	0.7563
R_w	0.8259	0.8108	0.8557	0.6898	0.7158	0.7059	0.7067	0.7415
R_w^2	0.6821	0.6574	0.7322	0.4758	0.5124	0.4983	0.4994	0.5498

	V10.1	V10.2	V11	V12	V13	V14	V15	V16
R	0.8674	0.8592	0.8520	0.7870	0.8128	0.8040	0.8037	0.8392
R^2	0.7524	0.7383	0.7259	0.6194	0.6607	0.6465	0.6460	0.7043
R_w	0.8293	0.8348	0.8310	0.7947	0.8111	0.8031	0.8088	0.8293
R_w^2	0.6877	0.6969	0.6906	0.6315	0.6579	0.6450	0.6542	0.6877

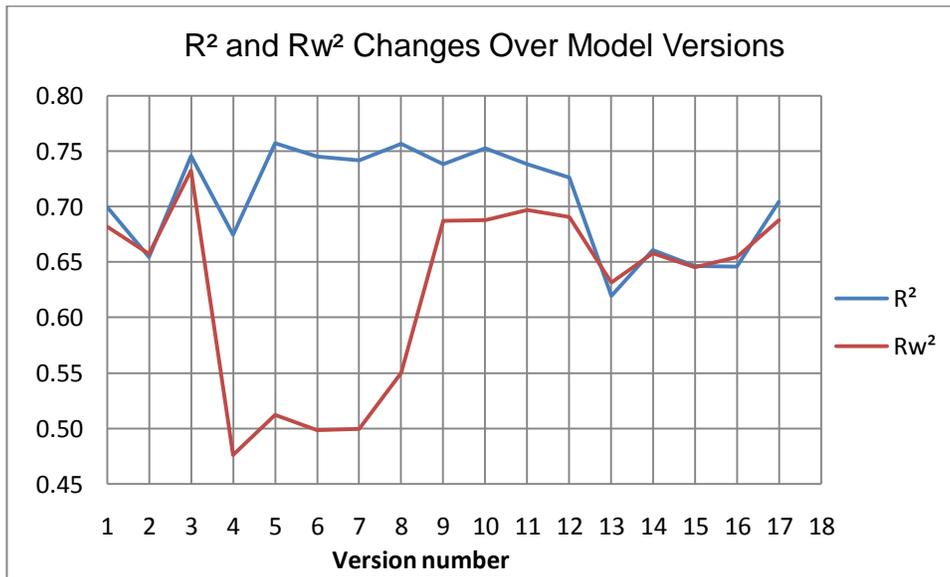


Figure 6.10 R and R_w values in each version

CHAPTER SEVEN

CONCLUSION AND DISCUSSION

7.1 CONCLUSION

The primary purpose of the study was to build a virtual watershed for the Shenandoah River Basin. The virtual watershed should be able to give reasonably accurate prediction of river discharge, which is important in decision making on water quantity related subjects.

River discharge is generated by sequences of physical processes, controlled by forcing such as weather and watershed characteristics such as soil/rock types. In hydrological models, these watershed characteristics are expressed as parameters, while the physical processes are expressed in mathematical equations. Therefore, a specific watershed should have a unique parameter set, which can best represent the watershed characteristics and simulate river flow.

To predict the future river discharge, this unique parameter set needs to be identified. In order to obtain this parameter set, one need to use existing discharge observations to calibrate the model. Therefore, the main objective for this study was model calibration.

To fulfill the main task, the distributed watershed modeling environment SWAT was employed for watershed model building, and the automatic parameter estimation tool PEST was employed for model calibration. The SWAT tool was modified as iSWAT for better groundwater simulation. The original linear-reservoir algorithm for groundwater (baseflow) was modified into a nonlinear form,

adding a new groundwater Beta parameter. PEST is coupled with SWAT, automatically calibrating the SWAT parameter values.

In the model calibration processes, parameters such as: 1) roughness coefficients (both for main channels and the tributaries), 2) baseflow parameters (groundwater delay, alpha and beta parameters), 3) soil parameters (subsurface flow length), 4) evapotranspiration parameters (canopy and efficiency), are automatically calibrated in PEST. To calibrate the derivatives of the objective function with respect to each adjustable parameter, PEST usually calls the model two times the number of adjustable parameters in one optimization iteration. For this iSWAT model, PEST carried out as many as 20 iterations to reach the minimum value of the objective function.

Including more parameters in a model can improve model performance. It is possible that the overall R^2 may not change much, better fit can be observed from the matching of baseflow, flow trend and recession. The cost for adding more parameters is more time and computational workload. In addition, a large number of parameters can cause problems with non-unique solutions, irrational parameters, and parameters that lack physical meaning.

Assigning observation weightings is an important part of the PEST calibration process. Different weighting methods were experimented: equal weights, inverse of mean discharge, inverse of standard deviation, and an ordinal scale method based on the stream network. The ordinal scale weighting method shows the best fitting results, greatly improving R^2 and NSE, compared to earlier attempts.

When a reliable method is available, pre-calibration of some parameters may help in reducing calibration time. Reducing the parameter space would improve model stability. While keeping these parameters unchanged, PEST can explore more possible values for other parameters, thus may result in better simulation results. Moreover, fixing more parameters would reduce the number of times PEST calls iSWAT, thus reducing the computational time.

Generally speaking, model calibration is not a simple process. One needs to explore different methods to generate a better hydrologic model.

The best Shenandoah Watershed model has R^2 of 0.7044, with 52 free parameters for the 7621.16 km^2 watershed incorporating 28 subbasins and 498 Hydrologic Response Units. The Beta parameter values for all the soil type within the area are approximate 0.43, which is close to Wittenberg's (1994) result of 0.5.

As a conclusion, recommendations for calibrating the iSWAT Shenandoah Model are:

- 1) Groundwater, evaporation and canopy parameters should be included as adjustable parameters in the model. These parameters should be classified by soil types and land use in order to keep the adjustable parameters to a reasonable number.
- 2) Roughness coefficients for the main channel should be calculated with GIS analysis and empirical equations, not adjusted in calibration.
- 3) Observation weights should be assigned according to the stream network and use the ordinal-scale weighting method.

7.2 FUTURE RESEARCH

This iSWAT model generally can simulate the river discharge in a reasonably good manner. However, there is still space for improvements.

1) Better application of PEST

PEST is a very powerful tool in parameter estimation. In this study, only the most basic function of PEST was utilized although other functions were briefly explored. Future work can concentrate on PEST's advanced regularization, together with its SVD-Assist tool. By employing such tool packages and setting proper constraints to the model, the parameter estimation process can be more efficient.

2) Systematically change certain parameter values

Feyereisen (2005) did a sensitivity analysis for SWAT input parameters. In his research, CN2 (curve number) for crop and forest land use are the most sensitive parameters in predicting total water yield in the 10-year period, stream flow and baseflow. Lenhart (2002) did similar research on SWAT parameter sensitivity using two analyzing methods. He found that the most sensitive parameters for hydrology and water quality are the physical soil properties such as bulk density and hydraulic conductivity. Curve number also showed a high sensitivity.

Garen (2005) pointed out that the curve number (CN) method of the Natural Resources Conservation Service is not properly used in many hydrological

models. Many modelers misunderstand the definition of overland flow with stream flow, which CN method is designed for. They also ignore the overflow generated from Saturation Excess, which is not included in SWAT model. Therefore, he suggested future modification of CN method in Hydrological Modeling.

White (2009) achieved better SWAT performance by using initial abstraction $I=0.05S$ instead of $0.2S$, and adjusting curve number based on the level of soil saturation in low-lying riparian zones. Easton (2007) included variable source areas (VSA) for runoff calculation and developed a SWAT-VSA version. Wang (2008) developed a Modified Curve Number method (MCN). They both improved model performance.

Therefore, there are still imperfections within the SWAT modeling environment. Modification of SWAT input parameters and process equations may greatly affect model output and lead to better predictions. Future works may include systematically changing parameters such as CN_2 , hydraulic conductivity, or modifying how parameters such as soil type and bulk density can be generated/ obtained.

3) Finer scaled DEM and soil map

Chaplot (2005) has made a study on how the resolution of Digital Elevation Model and Soil Maps would affect the ArcSWAT-generated SWAT model input and output. He used a DEM size of 20m and soil map scale of 1/25,000 as the base model, whose model output are used for comparison. He then

experimented with DEM size from 20m to 500m and soil map scale from 1/25,000, 1/250,000 to 1/500,000. Different DEM sizes result in different estimation of elevation above streams, channel lengths, watershed delineation and watershed area. Soil maps on different scales lead to different soil composition of the subwatershed, thus resulting differences soil type for each HRU and the percentage of a certain soil in the whole subbasin. SWAT outputs showed differences in the mean discharge, mean sediment and nitrogen transport in an 8-year period simulation. Results show that both DEM size and Soil Map Scale affect the model results. Moreover, Chaplot (2005) points out that HRU size may also affect results. He used a 3-hectare HRU in his study. He suggested that increasing/decreasing the HRU size may change the conclusions.

His research can explain the different channel lengths and slopes discussed in chapter 5.3. Using a finer DEM and soil map may improve this iSWAT performance. However, experimenting different data resolution can be time consuming; the whole model development process would need to be redone. Trying different data resolution and studying the parameter estimation results can be a good topic for future study.

4) Regrouping the parameters

The 16 Shenandoah calibrations show improvement in model performance over different approaches. However, there are still poorly performed reaches even in the best model Version 16.

From version 3m to version 16, reach 19's performances are always poor (Figure 7.1). The problems are shown in recession and baseflow. Modeled outputs from different model versions show generally over estimation of discharge. The modeled baseflow cannot be lowered where natural baseflow decreases.

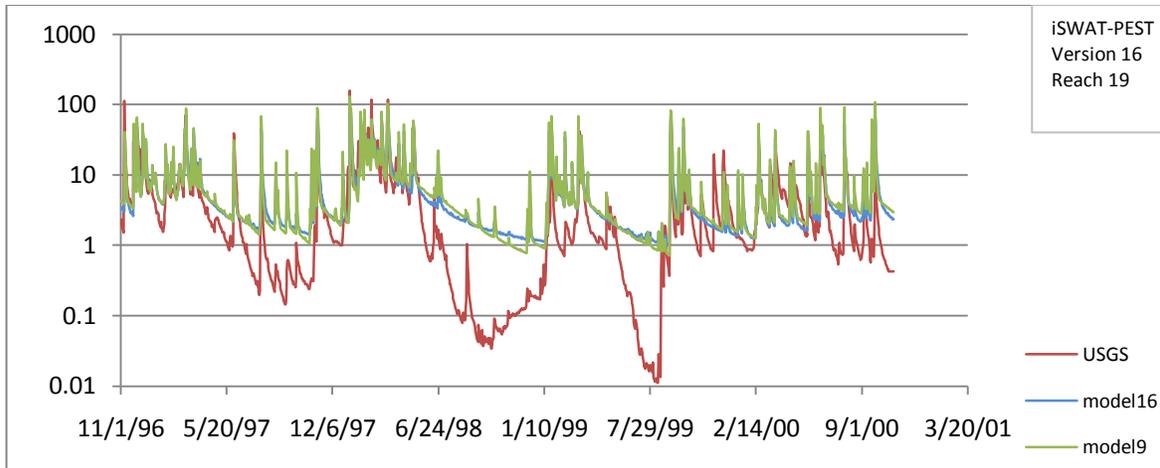


Figure 7.1 Hydrograph for reach 19 in Version 16

Most parameters in this Shenandoah Watershed Model are assigned by soil type. Roughness coefficients for tributaries are determined by dominant soil in the subbasin. Groundwater parameters are assigned by dominant soil type in each HRU (Table 4.1). There are three types of soil in reach 19, col (colluvium from sandstone, siltstone, and some shale), sss (shale, siltstone and fine grained sandstone), and san (sandstone), among which col is the dominant soil in the subbasin (Table 5.6).

Assuming that the parameters assigned to reach 19 are incorrect, other reaches that have similar soil formation would also perform poorly. However, reach 7 and reach 13, having similar soil type with reach19, show improving

performances over different calibrations while reach 19 is still poor in simulation.

These results indicate that the assignment of parameters by soil type might be improper. Reach 19 is located in mountainous regions. The great land slope could result in differences in flow recession simulation. On the other hand, the dominant soil type along rivers can be different from soil type in mountains, and the later soil happens to be the dominant soil in the subbasin. If it is true, then the simulation results can be greatly affected.

Therefore, the solution for the poorly performed reach might be re-designation of parameters. Parameters may not only depend on soil types, but also be taken into account the regional characteristics. Another solution can be reclassification of HRUs. It is possible that finer division of HRU would lead to more accurate simulation results.

7.3 LESSONS LEARNED

The thesis research has provided the opportunity to learn about many aspects of Water Resources Engineering, including hydrology, statistics, and modeling.

Precipitation and solar energy serves as the driving force in hydrologic cycle. Water from precipitation is retained by vegetation interception, directly evaporated or transpired by plants. Water infiltrates into soil, changing soil water content, contributing to groundwater storage and flow. The remaining part of water generates surface runoff, which goes directly into surface waterbodies

such as rivers and oceans. The whole process depends on rainfall, temperature, soil characters, land topography and land use.

Statistics is a very important tool in hydrologic modeling. Statistical test and coefficients are important criteria for evaluating model performance. However, due to the complexity of hydrologic models, it should be noted that evaluation of a model should not depend only on numerical measures. The realism of physical processes, rationality of parameters, and subjective judgment should also be taken into account.

In watershed modeling, many helpful software packages and tools are available to improve model performances. Optimization tools such as PEST can be used to perform automatic calibrations. GIS data are employed to estimate parameter values and reduce the number of free parameters. It should be kept in mind to use available information and tools in a smart way.

Consistency and patience are the keys in modeling. One should be continually tuning the model until it gives out the needed results for its intended use in management, planning, and design. Active and creative thinking is also of importance. Model modification should be done in an efficient and effective way.

APPENDIX A SWAT INPUT FILES LIST

Level	File type	Descriptions
watershed	file.cio	Master watershed file. This required file contains the names of watershed level files and parameters related to printing.
	.fig	Watershed configuration file. This required file defines the routing network in the watershed and listed input file names for different objects in the watershed
	.bsn	Basin input file. This required file defines values or options used to model physical processes uniformly over the entire watershed.
	.pcp	Precipitation input file. This optional file contains daily measured precipitation for a measuring gage. Up to 18 precipitation files may be used in each simulation and each file can hold data for up to 300 stations.
	.tem	Temperature input file. This optional file contains daily measured max and min temperature for a measuring gage. Up to 18 precipitation files may be used in each simulation and each file can hold data for up to 150 stations.
	.slr	Solar radiation input file. This optional file contains daily solar radiation for a measuring gage. The solar radiation file can hold data for up to 300 stations.
	.wnd	Wind speed input file. This optional file contains daily average wind speed for a measuring gage. The wind speed file can hold data for up to 30 stations.
	.hum	Relative humidity input file. This optional file contains daily relative humidity values for a measuring gage. This file can hold up to 300 stations
	.pet	Potential evapotranspiration input file. This optional file contains daily PET values for the watershed.
	.cst	Weather forecast input file. Optional
	.cal	Auto-calibration input file. Optional
	crop.dat	Land cover/plant growth database file. This required file contains plant growth parameters for all land covers simulated in the watershed.
	till.dat	Tillage database file. This required file contains information on the amount and depth of mixing caused by tillage operations simulated in the watershed
	pest.dat	Pesticide database file. This required file contains information on mobility and degradation for all pesticides simulated in the watershed.
	fert.dat	Fertilizer database file. This required file contains information on the nutrient content of all fertilizers and manures simulated in the watershed.
	urban.dat	Urban database file. This required file contains information on the building-up/ wash-off of solids in urban areas simulated in the watershed.

subbasin	.sub	Subbasin input file. This required file for each subbasin defines climatic inputs, tributary channel attributes, and the number and types of HURs in the subbasin.
	.wgn	Weather generator input file. This required file contains the statistical data needed to generate representative daily climatic data for a subbasin.
	.pnd	Pond/wetland input file. Optional
	.wus	Water use input file. Optional
	.rte	Main channel input file. This required file contains parameters governing water and sediment movement in the main channel of a subbasin
	.wwq	Watershed water quality input file. Optional
	.swq	Stream water quality input file. Optional
HRU	.hur	HRU input file. Required file for HUR level parameters. Catch-all file.
	.mgt	Management input file. This required file contains management scenario and specifies the land cover simulated in the HRU.
	.sol	Soil input file. This required file contains information about initial nutrient and pesticide levels of the soil in the HRU.
	.chm	Soil chemical in put file. Optional
	.gw	Groundwater input file. This required file contains information about the shallow and deep aquifer in the subbasin.
	.res	Reservoir input file. Optional
	.lwq	Lake water quality input file. Optional

APPENDIX B STUDY RECORDS

Part 1 Summary of Major Works

From January, 2010 to February, 2011, I have carried out several experimental versions of the Shenandoah iSWAT model. Here is a summary of differences of model set up in each version, model results for each version and where each version and its outputs are documented.

Version 1

Objective: A single executable program iSWAT was used to test if this self-compiled version of SWAT could run.

Results: The iSWAT model ran well.

Folders: 2010-01-20

Version 2

Objective: PEST was applied in combination with SWAT to ensure the parameter calibration process can be completed.

Parameters included: SURLAG (Surface runoff coefficient), 1;

n1 (Manning's n value for tributary channels), 5;

n2 (Manning's n value for main channels), 5

Results: PEST ran well in the estimation process. Total 5 optimizations with model called 86 times.

Folders: 2010-01-26 to 2010-02-05; SHEN_ALL_SWATCalib_V2

Version 3

Objective: Including new parameters in PEST to improve the performances of SWAT.

Parameters included: SURLAG (Surface runoff coefficient), 1;

n1 (Manning's n value for tributary channels), 5;

n2 (Manning's n value for main channels), 5

gd (Groundwater delay), 7;

a (Baseflow Alpha parameter), 7;

b (Baseflow Beta parameter), 7

Results: The adding of new parameters improved the model performances in catching the summer low flow. Total 4 optimizations with model called 168 times.

Folders: 2010-02-20; SHEN_ALL_SWATCalib_V3

Version 3m

Objective: Including new parameters in PEST to improve the performances of SWAT.

Parameters included: SURLAG (Surface runoff coefficient), 1;

n1 (Manning's n value for tributary channels), 5;

n2 (Manning's n value for main channels), 5

gd (Groundwater delay), 7;

a (Baseflow Alpha parameter), 7;

b (Baseflow Beta parameter), 7

e (Soil evaporation compensation factor), 10;
s (Slope length for lateral subsurface flow), 10;
epco (Plant uptake compensation factor), 2(Forest and crop field);
can (Maximum canopy storage), 2(Forest and crop field)

Results: The adding of new parameters improved the model performances in catching the summer low flow. Total 20 optimizations with model called 2237 times.

Note: This version was carried out after Version 16. This version is developed to include all the adjustable parameters while keeping them equally weighted. Therefore, the results can be compared to other versions which include all adjustable parameters but in different weighting methods (V6, V7, V8, V9).

Folders: 2011-03-02; SHEN_ALL_SWATCalib_V3m

Version 4

Objective: Change the weighting of each observation to improve model performance.

Parameters included: SURLAG (Surface runoff coefficient), 1;
n1 (Manning's n value for tributary channels), 5;
n2 (Manning's n value for main channels), 5
gd (Groundwater delay), 7;
a (Baseflow Alpha parameter), 7;
b (Baseflow Beta parameter), 7

Weighting method: Each observation group contributes to the sum of squared residuals differently. Use the inverse of their contributions to create new weighing factors for each group.

Results: Improvement in both high/low flow and recession. Total 14 optimizations with model called 838 times.

Folders: 2010-03-03; SHEN_ALL_SWATCalib_V4

Version 5 (Modified)

Objective: Add soil and ET parameters to provide better fit.

Parameters included: SURLAG (Surface runoff coefficient), 1;

n1 (Manning's n value for tributary channels), 5;

n2 (Manning's n value for main channels), 5

gd (Groundwater delay), 7;

a (Baseflow Alpha parameter), 7;

b (Baseflow Beta parameter), 7;

e (Soil evaporation compensation factor), 10;

s (Slope length for lateral subsurface flow), 10;

epco (Plant uptake compensation factor), 2(Forest and crop field);

can (Maximum canopy storage), 2(Forest and crop field)

Results: Total 14 optimizations with model called 1549 times. R=0.7158

Folders: 2010-05-26; SHEN_ALL_SWATCalib_V5Mod

Version 6

Objective: Change the weighting of each observation to improve model performance.

Parameters included: SURLAG (Surface runoff coefficient), 1;
n1 (Manning's n value for tributary channels), 5;
n2 (Manning's n value for main channels), 5
gd (Groundwater delay), 7;
a (Baseflow Alpha parameter), 7;
b (Baseflow Beta parameter), 7;
e (Soil evaporation compensation factor), 10;
s (Slope length for lateral subsurface flow), 10;
epco (Plant uptake compensation factor), 2(Forest and crop field);
can (Maximum canopy storage), 2(Forest and crop field)

Weighting method: Use the inverse of average discharge over the 13 year period for each observation group.

Results: Total 11 optimizations with model called 1203 times. R=0.7059

Folders: 2010-01-10; SHEN_ALL_SWATCalib_V6

Version 7

Objective: Reclassify the geographic information for each sub-watershed.

Parameters included: SURLAG (Surface runoff coefficient), 1;
n1 (Manning's n value for tributary channels), 6;

n2 (Manning's n value for main channels), 5
gd (Groundwater delay), 7;
a (Baseflow Alpha parameter), 7;
b (Baseflow Beta parameter), 7;
e (Soil evaporation compensation factor), 10;
s (Slope length for lateral subsurface flow), 10;
epco (Plant uptake compensation factor), 2(Forest and crop field);
can (Maximum canopy storage), 2(Forest and crop field)

Method: Collect information about the soil types and their percentage in each subarea. Define the dominant soil in the area (First by percentage; where similar percentage by physical location of stream network). By assigning Manning's n value for tributary channels by the dominant soil type, we add a parameter n1_cry and changed some n1 values in each reach. R=0.7067

Results: Total 10 optimizations with model called 993 times. The model performance is worse than the previous version.

Folders: 2010-05-26; SHEN_ALL_SWATCalib_V7; Documentation, geo-info.

Version 8

Objective: Change weighting method to improve model performance.

Parameters included: SURLAG (Surface runoff coefficient), 1;

n1 (Manning's n value for tributary channels), 6;

n2 (Manning's n value for main channels), 5
gd (Groundwater delay), 7;
a (Baseflow Alpha parameter), 7;
b (Baseflow Beta parameter), 7;
e (Soil evaporation compensation factor), 10;
s (Slope length for lateral subsurface flow), 10;
epco (Plant uptake compensation factor), 2(Forest and crop
field);
can (Maximum canopy storage), 2(Forest and crop field)

Weighting method: Each reach has its own mean discharge and standard deviation. Use the inverse of their S_d to eliminate the errors due to sample range.

Results: Total 11 optimizations with model called 1109 times. The overall R-square improved. Reach 13 has better output, but others no much effects.

R=0.7415

Folders: 2010-06-23; SHEN_ALL_SWATCalib_V8

Version 9

Objective: Change weighting method to improve model performance.

Parameters included: SURLAG (Surface runoff coefficient), 1;

n1 (Manning's n value for tributary channels), 6;
n2 (Manning's n value for main channels), 5
gd (Groundwater delay), 7;

a (Baseflow Alpha parameter), 7;
b (Baseflow Beta parameter), 7;
e (Soil evaporation compensation factor), 10;
s (Slope length for lateral subsurface flow), 10;
epco (Plant uptake compensation factor), 2(Forest and crop field);
can (Maximum canopy storage), 2(Forest and crop field)

Weighting method: From the most upstream reaches to the most downstream reaches, we rank them from 1 to 12. The new weightings are the inverse of their rank. This is actually another way of taking into account the mean discharge differences.

Results: Total 7 optimizations with model called 1228 times. The overall R-square improved 13%. The parameter values differ a lot with the previous version. R=0.8291

Folders: 2010-07-02; SHEN_ALL_SWATCalib_V9

Version 10

Objective: Have n1 and n2 values fixed and see how PEST would change other parameters.

Parameters included: SURLAG (Surface runoff coefficient), 1;
n1 (Manning's n value for tributary channels), 6, fixed;
n2 (Manning's n value for main channels), 5, fixed;
gd (Groundwater delay), 7;

a (Baseflow Alpha parameter), 7;
b (Baseflow Beta parameter), 7;
e (Soil evaporation compensation factor), 10;
s (Slope length for lateral subsurface flow), 10;
epco (Plant uptake compensation factor), 2(Forest and crop field);
can (Maximum canopy storage), 2(Forest and crop field)

Method: Version10.1, the fixed n values are assigned the very first values of 0.07;

Version10.2, the fixed n values are assigned the average values of V7, V8 and V9.

Results: Total 10 optimizations with model called 705 times. Both the versions have a R-square of 0.7. It seems that roughness coefficients has little effect on the model performance.

Folders: 2010-07-18; SHEN_ALL_SWATCalib_V10.1

2010-07-26; SHEN_ALL_SWATCalib_V10.2

Version 11

Objective: Use empirical equations to re-evaluate Manning's roughness coefficients for main channels.

Parameters included: SURLAG (Surface runoff coefficient), 1;

n1 (Manning's n value for tributary channels), 6, fixed;

n2 (Manning's n value for main channels), 28, fixed;

gd (Groundwater delay), 7;

a (Baseflow Alpha parameter), 7;
b (Baseflow Beta parameter), 7;
e (Soil evaporation compensation factor), 10;
s (Slope length for lateral subsurface flow), 10;
epco (Plant uptake compensation factor), 2(Forest and crop field);
can (Maximum canopy storage), 2(Forest and crop field)

Method: Use ArcGIS to evaluate areas of each sub-watershed, the lengths of each main channel. Use empirical equations to recalculate n values and have them applied to the model.

Results: Total 15 optimizations with model called 1932 times. This version has an R-square of 0.6906.

Folders: 2010-09-06; SHEN_ALL_SWATCalib_V11; GIS

Version 12 (overlooked sub-basin area)

Objective: Change input files, use new channel lengths and slopes. Keep the n values the same as the previous version.

Parameters included: SURLAG (Surface runoff coefficient), 1;
n1 (Manning's n value for tributary channels), 6;
n2 (Manning's n value for main channels), 28, fixed;
gd (Groundwater delay), 7;
a (Baseflow Alpha parameter), 7;
b (Baseflow Beta parameter), 7;

e (Soil evaporation compensation factor), 10;
s (Slope length for lateral subsurface flow), 10;
epco (Plant uptake compensation factor), 2(Forest and crop field);
can (Maximum canopy storage), 2(Forest and crop field)

Method: Use ArcGIS to evaluate areas of each sub-watershed, the lengths of each main channel. Change the main channel length and slope in each .rte file.

Results: Total 3 optimizations with model called 268 times. This version has an R-square of 0.6315. Although the results are not as good as V11, this model is more reasonable.

Folders: 2010-10-22; SHEN_ALL_SWATCalib_V12

Version 13

Objective: Use provided channel information to recalculate n values. Keep original input files unchanged.

Parameters included: SURLAG (Surface runoff coefficient), 1;
n1 (Manning's n value for tributary channels), 6;
n2 (Manning's n value for main channels), 28, fixed;
gd (Groundwater delay), 7;
a (Baseflow Alpha parameter), 7;
b (Baseflow Beta parameter), 7;
e (Soil evaporation compensation factor), 10;

s (Slope length for lateral subsurface flow), 10;
epco (Plant uptake compensation factor), 2(Forest and crop
field);

can (Maximum canopy storage), 2(Forest and crop field)

Method: Use channel details in the input files and use the empirical equation to
recalculate the n values. Use the new n values in the pest control file.

Keep the original input data unchanged.

Results: Total 7 optimizations with model called 756 times. This version has a R-
square of 0.6579.

Folders: 2010-11-28; SHEN_ALL_SWATCalib_V13

Version 14 (new regularization mode)

Objective: Use the up-to-date information of this model to redo the PEST
regularization calculation.

Results: Total 2 optimizations with model called 147 times. This version has an R
of 0.8149.

Folders: 2010-11-30; SHEN_ALL_SWATCalib_V14

Version 15 (new prediction mode)

Objective: Use the up-to-date information of this model to redo the PEST
prediction calculation.

Results: Total 4 optimizations with model called 353 times. This version has a R-
square of 0.6579.

Folders: 2011-02-01; SHEN_ALL_SWATCalib_V15

Version 16

Objective: One final version of iSWAT-PEST.

Parameters included: SURLAG (Surface runoff coefficient), 1;

n1 (Manning's n value for tributary channels), 6;

n2 (Manning's n value for main channels), 28, fixed;

gd (Groundwater delay), 7;

a (Baseflow Alpha parameter), 7;

b (Baseflow Beta parameter), 7;

e (Soil evaporation compensation factor), 10;

s (Slope length for lateral subsurface flow), 10;

epco (Plant uptake compensation factor), 2 (Forest and crop field);

can (Maximum canopy storage), 2 (Forest and crop field)

Method: One final version including all adjustable parameters, using new

Manning's n values for main channels, changing all information

regarding channel length and slope in input files, applying the ordinal

weighting method.

Results: Total 23 optimizations with model called 2402 times. This version has an

R-square of 0.6579.

Folders: 2011-02-22; SHEN_ALL_SWATCalib_V16

Part 2 Problem Encountered

Groundwater storages in Version 5(original one) were incorrect. Deep aquifer storages were intended to be set as a constant 1000 inches and the initial shallow aquifer storage be 1000 inches. No percolation from SA to DA was planned to be modeled. However, in the original version5, initial value for SA storage is 0.5 inch and percolation rate is 0.05. (Folders: 2010-03-15; SHEN_ALL_SWATCalib_V5)

The problem was caused by incorrect .gwi files. Since the .gwi files were written by the pest template files, the errors in gw*.ptf were the ultimate causes.

This version was corrected as the Modified Version 5. All groundwater components (storage and flux) performed as expected.

Part 3 Other Endeavors

1. Application of SENSAN in PEST Package.

Objective: Subjectively optimize of the model parameters.

SENSAN is a tool used to do sensitivity analysis. For each parameter set, only one run is needed. Actually, this tool is used for changing one or more

parameters in the model to calculate the sensitivity of the parameters. We just used this tool to re-write all files needed in SWAT and give output files (Folders: sensan).

One analysis package was designed to automatically generate comparisons of calculated values and observations (Folders: 2010-04-01 SENSAN).

By manually adjust the parameters related to recessions, high flow and low flows, better model performances were observed. The whole set of information include parameter names, meanings, ranges, changes made in different trials, results for each trial and comments on the results. They are recorded in the para_rec.docx file.

2. Application of the results from SENSAN in PEST

Objective: Through the subjective process of SENSAN, we found that some of the parameters are of special importance to the model. Thus, we set these parameters fixed and adjusted the range of other parameters in the pest control file. Then let PEST do the parameter estimation again. This process was actually manually minimizing the number of parameters and decreasing the changing range. (Folders: 2010-04-10 sensan-pest-1)

Results: The results were not as good as expected. It showed that the model was so complex that a change in one parameter could result in changes in many aspects of the model output.

3. Seeking solutions in PEST

3.1 Change the methods of different weighting.

New weighting method: Use the inverse of the average runoff for each reach (the 15 reaches that observations are available).

Results showed improvements in model performance (Folders: 2010-04-14)

Other weighting methods under consideration: 1) Standard deviation of each reach

2) Coefficient of variation (σ/μ)

These methods were not tried due to the discovery of the errors in the original model version 5.

All new weights were recorded in the new weights.exl.

3.2 Using Regularization Mode in PEST

In regularization mode, PEST aims to maximize adherence to a certain “regularization condition” (by minimizing a regularization objective function) while ensuring that the measurement objective function rises no higher than a specified level. Reach 13 was always the most problematic one. Therefore, we set this particular observation group as the regularization group required by PEST. Rerun the model.

The results showed no much difference with calculation in the estimation mode of PEST.

Folders: 2010-04-19

3.3 Using Prediction Mode in PEST.

In predictive analysis mode, PEST aims to maximize or minimize a specified prediction while maintaining the model in a calibrated state (ensuring that the objective function rises no higher than a specified level). Reach 13 showed generally large underestimation of runoff. Therefore, we set one most deviate observation in reach 13 as a single observation group “predict” as required by the PEST Prediction Mode. PEST was asked to maximize the calculated value of this group while keeping a relatively high level of significance in the objective function. The results showed no much difference with calculation in the estimation mode of PEST.

Folders: 2010-04-20

4. Application of GIS in Estimating Manning’s Roughness Coefficients

Objective: To get more accurate roughness coefficients. The regional regression equations were employed. The basic concept is to use Manning’s Equation calculating the roughness coefficient. A more detailed report on this topic is in Folders: GIS, n_Evaluation.

Part 4 Notes for Other Folders

1. 2010-03-15 seasonal analysis: This folder contains the information of seasonal analysis of the original model version 5. Calculated runoff in summer showed more obvious under-estimation; the values in other seasons were more or less

the same with observations. This analysis was aim at identifying one way to improve model performance.

2. 2010-04-21 GW veri: This folder includes the information about groundwater analysis of original version 5. It was from these files that we noticed the unusual performance of DA and SA storages.

3. 2010-04-24 new weight-2: uncompleted due to the discovery of the errors in version 5.

4. 2010-05-21 DA_SA check: This folder contains all hru information calculated in version 4. The check of DA and SA storage in version 4 showed that the .gwi files in V4 were correct. This analysis led to the correction of gwi*.ptf in V5-modified.

5. 2010-08-08 GIS: This folder contains the information how new Manning's n values (for the main channels) are calculated. In the folder is the GIS layers and spreadsheet for calculating. The results of this evaluation showed that the n value for each reach differs even if they are assigned the same soil type. Further study is needed to check the accuracy of the calculation and how we can put the results into use in iSWAT model.

REFERENCES

Ayyub, B. M. and R. H. McCuen, 1997. Probability, Statistics, and Reliability for Engineers. New York: CRC Press.

Baffaut, C. and V. Benson. 2008. Possibilities and challenges for modeling flow and pollutant transport in a karst watershed with SWAT. Paper No. 083933. St. Joseph, Mich.: ASABE.

Baginska, B., W. Milne-Home, and P.S. Cornish, 2003. Modeling nutrient transport in Currency Creek, NSW with AnnAGNPS and PEST. *Environmental Modelling & Software*, 18:801-808.

Bekele, E. G. and J. W. Nicklow, 2007. Multi-objective automatic calibration of SWAT using NSGA-II. *Journal of Hydrology*, 341:165-176.

Butcher, J. 2008. "Watershed Modeling",
<http://www.epa.gov/owow/watershed/wacademy/acad2000/modeling/model.htm>
(Accessed Nov. 2010)

Chaplot, V. 2005. Impact of DEM mesh size and soil map scale on SWAT runoff, sediment, and NO₃-N loads predictions. *Journal of Hydrology*, 312:207-222.

Cho, J. and S. Ha. 2010. Parameter optimization of the QUAL2K model for a multiple-reach river using an influence coefficient algorithm. *Science of the Total Environment*, 408:1985-1991.

Confesor, R. B. and G. W. Whittaker, 2007. Automatic calibration of hydrologic models with multi-objective evolutionary algorithm and pareto optimization.

Journal of the American Water Resources Association, Vol.43, No.4, August.

Connect Water, 2006. "Recession Analysis",

http://www.connectedwater.gov.au/framework/recession_analysis.php (Accessed Feb, 2011)

DeBarry, P. A. 2004. Watersheds: Processes, Assessment and Management, July 2004.

Doherty, J. 2004. PEST Model Independent Parameter Estimation User Manual: 5th Edition. Available online at <http://www.epa.gov/ceampubl/tools/pest>.

Doherty, J. and John M. Johnston, 2003. Methodologies for Calibration and Predictive Analysis of a Watershed Model. *Journal of the American Water Resources Association*, 39(2):251-265.

DC Water. "History – DC Water – District of Columbia Water and Sewer Authority". http://www.dcwater.com/about/gen_overview.cfm (Accessed 2010-09-28)

Duan, Q. H. , V. Gupta, S. Sorooshian, A. N. Rousseau, and R. Turcotte, 2002. Calibration of Watershed Models. Washington D.C: American Geophysical Union.

Easton, Z., D. Fuka, M. Walter, D. Cowan, E. Schneiderman, and T. Steenhuis, 2008. Re-conceptualizing the soil and water assessment tool (SWAT) model to predict runoff from variable source areas. *Journal of Hydrology*, 348(3/4):279-291.

Echegaray, G. A. 2009. Modification of the SWAT Model to Simulate Hydrologic Processes in a Karst-influenced Watershed. Master of Science, Biological Systems Engineering. Blacksburg, Virginia.

Eckhardt, K. and J.G.Arnold, 2001. Automatic calibration of a distributed catchment model. *Journal of Hydrology*, 251:103-109.

Fang, Q. , T. Green, L. Ma, R. Erskine, R. Malone, and L. Ahuja, 2010. Optimizing Soil Hydraulic Parameters in RZWQM2 under Fallow Conditions. *Soil Science Society of America Journal*, Vol.74, Num.6, November-December.

Feyereisen, G. W., T. Strickland, D. Bosch, and D. Sullivan, 2007. Evaluation of SWAT Manual Calibration and Input Parameter sensitivity in the Little River Watershed. *American Society of Agricultural and Biological Engineers*, 50(3):843-855.

Fontaine, T.A., T.S. Cruickshank, J.G. Arnold, and R.H. Hotchkiss, 2002. Development of a snowfall-snowmelt routine for mountainous terrain for the soil water assessment tool (SWAT). *Journal of Hydrology*, 262:209-223.

Garen, D. C. and D. S. Moore, 2005. Curve Number Hydrology in Water Quality Modeling: Uses, Abuses, and Future Directions. *Journal of the American Water Resources Association*, 41(2):377-388.

Griensven, A. V. and W. Bauwens, 2005. Application and evaluation of ESWAT on the Dender basin and the Wister Lake basin. *Hydrological Process*, 19:827-838.

Huang, Y. and L. Liu, 2010. Multiobjective Water Quality Model Calibration Using a Hybrid Genetic Algorithm and Neural Network–Based Approach. *Journal of Environmental Engineering*, Vol.136, No.10, October.

ICPRB, 2008. "Potomac Timeline"

http://www.potomacriver.org/cms/index.php?option=com_content&view=article&id=96&catid=39 (Accessed 2011-02-15)

ICPRB, 2010. "CO-OP History".

http://www.potomacriver.org/cms/index.php?option=com_content&view=article&id=98%3Aco-op-history&catid=47%3A drinking-water-supply&Itemid=122
(Accessed Feb.2011)

ICPRB, 2011a. "Facts & FAQs",

http://www.potomacriver.org/cms/index.php?option=com_content&view=article&id=70&Itemid=57 (Accessed in Feb, 2011)

ICPRB, 2011b. "Interstates Commission on the Potomac River Basin",

http://www.potomacriver.org/cms/index.php?option=com_content&view=article&id=170&Itemid=28 (Accessed in Feb, 2011)

ICPRB, 2011c. "Middle Potomac River Watershed Assessment > Project Details",

http://www.potomacriver.org/cms/index.php?option=com_content&view=article&id

d=163-sustainableflowssummary&catid=34-restore-enhance-conserve-protect
(Accessed in Feb, 2011)

ICPRB. "Land Use in Potomac River Basin",
http://www.potomacriver.org/info_center/maps/LandUse.pdf (Accessed Feb,
2011)

Immerzeel, W.W. and P. Droogers, 2008. Calibration of a distributed hydrological model based on satellite evapotranspiration. *Journal of Hydrology*, 349:411-424.

Iskra, I. and R. Droste 2007. Application of Non-Linear Automatic Optimization Techniques for Calibration of HSPF. *Water Environment Research: A Research Publication of the Water Environment Federation*, 79(6):647-659.

Islama, N., W. Wallender, J. Mitchell, S. Wicks, and R. Howitt, 2006. A comprehensive experimental study with mathematical modeling to investigate the affects of cropping practices on water balance variables. *Agricultural Water Management*, 82:129-147.

Kannan, N., C. Santhi, and J. G. Arnold, 2008. Development of an automated procedure for estimation of the spatial variation of runoff in large river basins. *Journal of Hydrology*, 359:1-15.

Kim, J. and Y. Park, D. Yoo, N. Kim, B. A. Engel, S. Kim, K. Kim, and K. Lim, 2009. Development of a SWAT Patch for Better Estimation of Sediment Yield in Steep Sloping Watersheds. *Journal of the American Water Resources Association*, 45(4):963-972.

Kim, N. and J. Lee, 2010. Enhancement of the channel routing module in SWAT. *Hydrological Process*, 24:96-107.

Lenhart, T., K. Eckhardt, N.Fohrer, and H.G. Frede, 2002. Comparison of Two Different Approaches of Sensitivity Analysis. *Physics & Chemistry of the Earth - Parts A/B/C*, 27(9/10):645.

Liu, Y., W. Yang, and X. Wang, 2008. Development of a SWAT extension module to simulate riparian wetland hydrologic processes at a watershed scale. *Hydrological Process*, 22:2901-2915.

Maidment, D. R., 1993. Handbook of Hydrology. McGraw-Hill Inc.

Marquardt, D. W. 1963. An Algorithm for Least-squares Estimation of Nonlinear Parameters. *Journal of the Society for Industrial and Applied Mathematics*, Vol.11, No. 2.

McCandless, T. L. 2003. Bankfull discharge and channel characteristics of streams in the AP/ VR hydrologic regions. U.S. Fish and Wildlife Service, CBFO-S03-01. Available online at www.fws.gov/r5cbfo

McCuen, R. H. 2005. Hydrologic Analysis and Design, 3/E. Prentice Hall.

McCuen, R. H., Z. Knight, and A. G. Cutter, 2006. Evaluation of the Nash-Sutcliffe Efficiency Index. *Journal of Hydrologic Engineering*, 11(6): 597.

McCuen, R.H., 2010. Class notes from ENCE 630.

Muleta, M. K. and J. W. Nicklow, 2005. Sensitivity and uncertainty analysis coupled with automatic calibration for a distributed watershed model. *Journal of Hydrology*, 306:127-145.

Nash, J.E. and J.V. Sutcliffe, 1970. River flow forecasting through conceptual models part I — A discussion of principles. *Journal of Hydrology*, 10(3):282-290.

Neitsch, S.L. J.G. Arnold, J.R. Kiniry, R.Srinivasan, and J.R. Williams, 2004. Soil and Water Assessment Tool Input/ Output File Documentation. September.

Neitsch, S.L., J.G. Arnold, J.R. Kiniry, and J.R. Williams, 2005. Soil and Water Assessment Tool Theoretical Documentation. January.

NOAA, 2011. "Hydrographs",
http://www.nws.noaa.gov/os/hod/SHManual/SHMan017_hydrograph.htm
(Accessed Mar. 2011)

NOAA-NCDC, 2009. "NCDC: National Climate Data Center",
<http://www.ncdc.noaa.gov/oa/ncdc.html> (Accessed Feb. 2010)

Official SWAT Web Site, 2010. "SWAT", <http://swatmodel.tamu.edu/> (Accessed Feb. 2010)

Potomac Watershed Partnership, 2008a. "Shenandoah River",
<http://www.potomacwatershed.net/ijourney/shenando/shenando.html> (Accessed in Feb, 2011)

Potomac Watershed Partnership, 2008b. "Washington D.C. Area", <http://www.potomacwatershed.net/ijourney/washdc/washdc.html> (Accessed in Feb, 2011)

Santanello, J. A., C. D. Peters-Lidard, M. E. Garcia, D. M. Mocko, M. Tischler, M. Susan Moran, and D.P. Thoma, 2007. Using remotely-sensed estimates of soil moisture to infer soil texture and hydraulic properties across a semi-arid watershed. *Remote Sensing of Environment*, 110:79-97.

Shultz, M. J. 2007. Comparison of Distributed Versus Lumped Hydrologic Simulation Models Using Stationary Moving Storm Events Applied to Small Synthetic Rectangular Basins and an Actual Watershed. Doctor of Philosophy, University of Texas, Arlington.

Soil Survey Staff, Natural Resources Conservation Service, United States Department of Agriculture. "Official Soil Series Descriptions". <http://soils.usda.gov/technical/classification/osd/index.html>. (Accessed Mar. 2011)

Southeast Regional Climate Center, 2010. "Woodstock 2 NE, Virginia- Climate Summary", <http://www.sercc.com/cgi-bin/sercc/cliMAIN.pl?va9263> (Accessed Mar. 2011).

SSP&A Inc. 2010. "PEST", <http://www.sspa.com/pest/> (Accessed Oct. 2010)

TAMU, 2010. "Hydrologic Models Inventory", <http://hydrologicmodels.tamu.edu/models.htm> (Accessed in Feb, 2011)

Thomas, William G., 2004. "The Shenandoah Valley", Southern Spaces, April 20, 2004, <http://southernspaces.org/2004/shenandoah-valley> (Accessed in Nov. 2010)

Tischler, M., M. Garcia, C. Peters-Lidard, M.S. Moran, S. Miller, D. Thoma, S. Kumar, and J. Geiger, 2007. A GIS framework for surface-layer soil moisture estimation combining satellite radar measurements and land surface modeling with soil physical property estimation. *Environmental Modelling & Software*, 22:891-898.

Tolson, B. A. and C. A. Shoemaker, 2007. Cannonsville Reservoir Watershed SWAT2000 model development, calibration and validation. *Journal of Hydrology*, 337:68-86.

University of Florida, 2007. "Glossary of Water Related Terms", <http://waterquality.ifas.ufl.edu/Glossary/Glossary.htm#Baseflow> (Accessed Feb. 2011)

US. EPA, 2009. "What is a watershed?" <http://water.epa.gov/type/watersheds/whatis.cfm> (Accesses Feb. 2011)

USGS, 2010a. "USGS Water Resources: Boundary Descriptions and Names of Regions, Subregions, Accounting Units and Cataloging Units" http://water.usgs.gov/GIS/huc_name.html (Accessed Nov. 2010)

USGS, 2010b. "WoWS FAQ",
http://wwwbrr.cr.usgs.gov/projects/SW_MoWS/faqs/faqs.shtml (Accessed Feb,
2011)

USGS, 2011a. "Hydrologic Unit Maps", <http://water.usgs.gov/GIS/huc.html>
(Accessed Feb. 2011)

USGS, 2011b. "Science in Your Watershed: Locate Your Watershed",
http://water.usgs.gov/wsc/map_index.html (Accessed Mar. 2011)

USGS, 2011c. "Science in Your Watershed",
<http://water.usgs.gov/wsc/acc/020700.html> (Accessed Mar. 2011)

Vazquez-Amabile, G. G. 2005. Use of SWAT to Compute Groundwater Table
Depth and Streamflow in the Muscatatuck River Watershed. *Transactions of the
ASAE*, 48(3):991-1003.

Wang, X. and A. M Melesse, 2005. Evaluation of the SWAT model's Snowmelt
Hydrology in a Northwest Minnesota Watershed. *Transactions of the ASAE*,
48(4):1359-1376.

Wang, X., and S. Shang, W. Yang, and A. M. Melesse, 2008. Simulation of
Agricultural Watershed Using an Improved Curve Number Method in SWAT.
Transactions of the ASABE, 51(4):1323-1339.

White, E. D., G. W. Feyereisen, T. L. Veith, and D. D. Bosch, 2009. Improving Daily Water Yield Estimation in the Little River Watershed: SWAT Adjustments. *Transactions of the ASABE*, 52(1):69-79.

White, E. D., Z. M. Easton, D. R. Fuka, A. S. Collick, E. Adgo, M. McCartney, S. B. Awulachew, Y. G. Selassie, and T. S. Steenhuis. 2010. Development and application of a physically based landscape water balance in the SWAT model. *Hydrological Process*. 25(6):915-925. (Published online, 8 Oct. 2010)

Wiese, B. and G. Nutzmann, 2009. Transient Leakance and Infiltration Characteristics during Lake Bank Filtration. *Groundwater*, 47(1):57-68.

Winchell, M., R. Srinivasan, M. Di Lusio, and J. Arnold, 2007. ArcSWAT Interface for SWAT, User's guide.

Wittenberg, H. and M. Sivapalan, 1999. Watershed groundwater balance estimation using streamflow recession analysis and baseflow separation. *Journal of Hydrology*, 219:20-33.

Xie, X. and Y. Cui, 2011. Development and test of SWAT for modeling hydrological processes in irrigation districts with paddy rice. *Journal of Hydrology*, 396:61-71.

Zheng, J. and Li G. Han Z., Meng G., 2010. Hydrological cycle simulation of an irrigation district based on a SWAT model. *Mathematical and Computer Modeling*, 51:1312-1318.